

Peridigm

Peridigm Installation Guide

For Peridigm versions $\geq 1.4.1$

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This document is part of the PeriDoX repository [1].

The complete repository can be found at:

<https://github.com/PeriDoX/PeriDoX>**Citing**

When citing this document, please reference the following:

Martin Rädcl, Christian Willberg, Peridigm Users Guide, DLR-IB-FA-BS-2018-23, DLR Report, 2018, in PeriDoX, DOI: [10.5281/zenodo.1403015](https://doi.org/10.5281/zenodo.1403015)**Disclaimer**

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1. About *Peridigm*

1.1. Description

Peridigm is an open-source computational peridynamics code developed at Sandia National Laboratories for massively-parallel multi-physics simulations. It has been applied primarily to problems in solid mechanics involving pervasive material failure. *Peridigm* is a C++ code utilizing foundational software components from Sandia's *Trilinos* project and is fully compatible with the Cubit mesh generator and *ParaView* visualization code.

Peridigm development began under the Physics & Engineering Models element of the US DOE's Advanced Simulation and Computing (ASC) program. The project was led by Michael Parks and managed by John Aidun. Subsequent funding has been provided by the US DOE through the ASC, ASCR, and LDRD programs.

1.2. Addresses

Official homepage: <https://peridigm.sandia.gov/>
Source code repository: <https://github.com/peridigm/peridigm>
Release snapshots: Must be requested via Download Registration Form on <https://peridigm.sandia.gov/content/download-registration-form>
User guide [2]: <http://www.sandia.gov/djlittl/docs/PeridigmV1.0.0.pdf>

1.3. Hardware requirements

Currently, there are no hardware requirements available or known. Publications, reports and presentations continuously mention the massive parallelization possible and presumably also necessary to run *Peridigm*.

Information on the performance of *Peridigm* on different system will be added as soon as it is available.

1.4. Features

1.4.1. Example 1

The simulation of impact and brittle fracture displayed in Figure 1.1 was achieved using explicit transient dynamics, the linear peridynamic solid constitutive model, short-range force contact, and a critical stretch bond failure law.

Peridynamics provides a natural framework for capturing pervasive material failure and fracture.

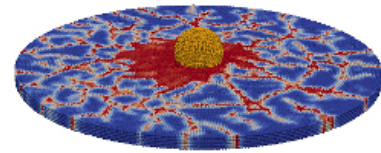


Figure 1.1.: Impact failure

1.4.2. Example 2

Peridigm is capable of performing explicit dynamic, implicit dynamic, and quasi-static time integration.

The tensile test simulation presented in Figure 1.2 was attained using an elastic correspondence constitutive model and quasi-static time integration. Pre- and post-processing were carried out using Sandia's *Cubit* mesh generator and *ParaView* visualization code.



Figure 1.2.: Tensile test

1.4.3. Example 3

The fragmentation of an expanding cylinder, shown in Figure 1.3, was simulated using the linear peridynamic solid constitutive model and critical-stretch bond failure rule. Initial velocities for each node in the discretization were specified via user-supplied analytic expressions.

Peridigm utilizes the RTCompiler function parser to process C-style expressions for the specification of input parameters, including initial and boundary conditions.

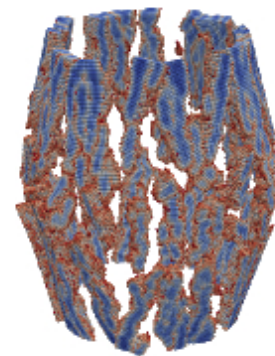


Figure 1.3.: Fragmentation

1.5. License

As of 04.02.2016 *Peridigm* is distributed under the three-term BSD license.

The current license terms can be obtained from:

<https://peridigm.sandia.gov/content/license>.

1.6. Peridigm working environment

Peridigm is a standalone tool for the handling of peridynamic models. Sandia National Labs suggests the use of *CUBIT* as the mesh generator and pre-processor and *ParaView* for post-processing. However, *CUBIT* is not publicly available free of charge except for U.S. government agencies. Any visualization package capable of reading and displaying ExodusII-format [3] data may be used to visualize the output of a *Peridigm* simulation. The creators of *Peridigm* use *ParaView*.

This installation guide focusses on the installation of the core program *Peridigm*. Several libraries are required as well as some basic tools *Peridigm* or one of its libraries is dependent on. All required tools for the use of *Peridigm* in a working environment are shown in Figure 1.4.

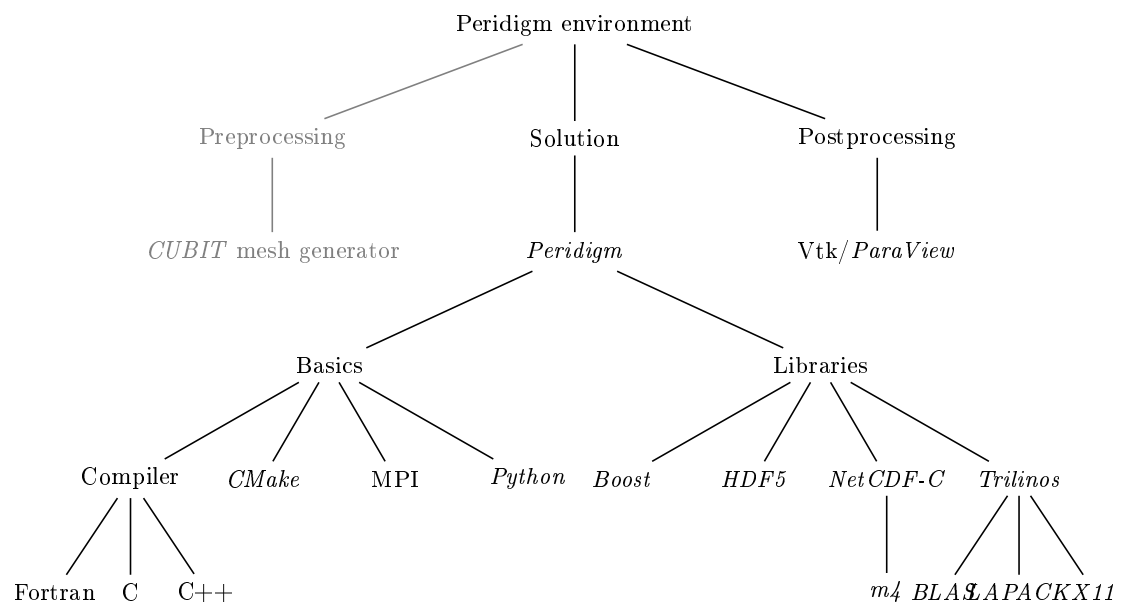
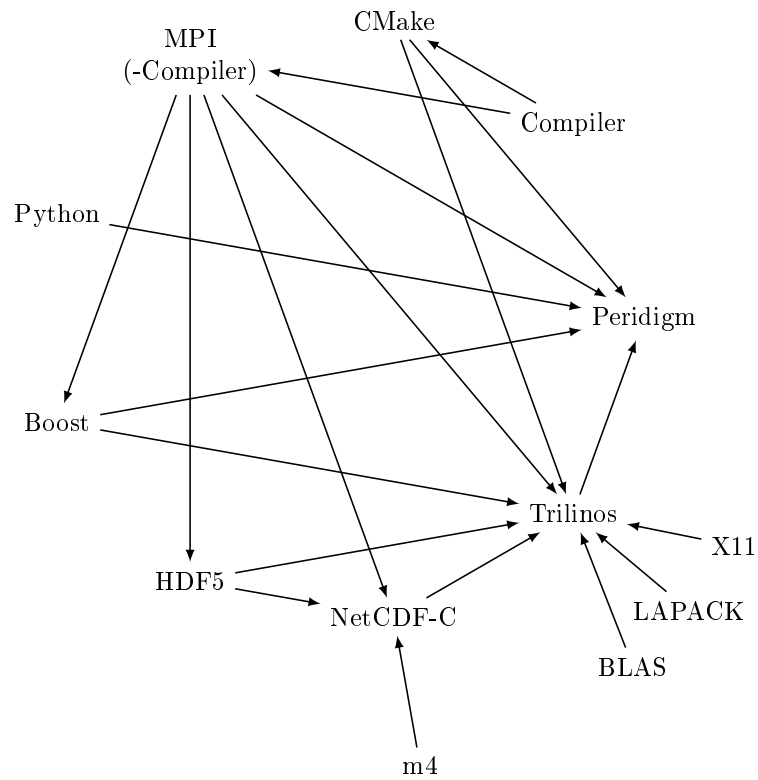


Figure 1.4.: Peridigm working environment tree

The installation guide features descriptions to the installation of all basic tools, libraries and *Peridigm* itself.

1.7. Dependencies

Below the dependencies between the individual tools and packages are shown.

Figure 1.5.: *Peridigm* package dependencies

2. Linux in a virtual machine

If no native Linux-based operating system is available on a device it is possible to install a Linux distribution inside a virtual machine. The device used to install the virtual machine in is called the host in the description.

In case you have a native Linux operating system on your device you can skip the following steps and go to chapter 3.

2.1. Download Linux Distribution

For *Peridigm* we need a Linux distribution for the installation inside the virtual machine. Here, *openSUSE* is used. To download the latest version of *openSUSE* go to:

https://en.opensuse.org/Main_Page

In the top bar of the homepage go to the download section and choose *Latest stable release*. On the newly loaded page choose to download the DVD image as installation medium and perform the download onto your device. Beware, the image is quite big.

2.2. Install the virtual machine

2.2.1. Download and install virtualization software

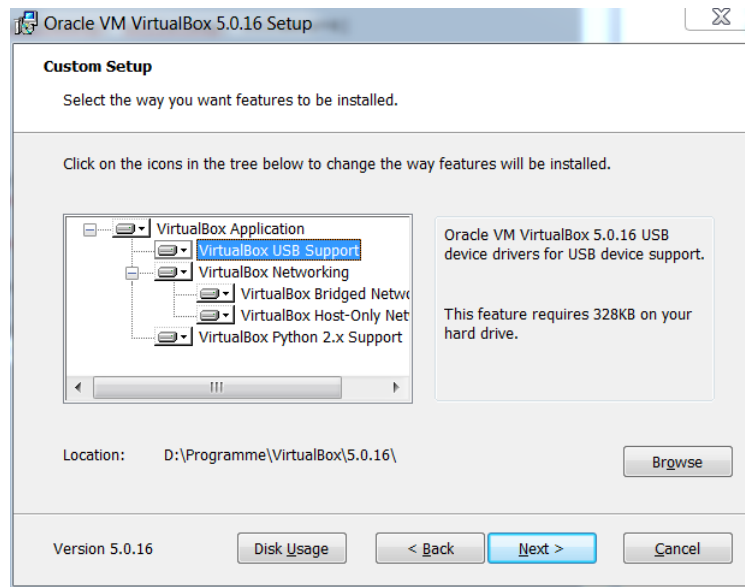
For the current case *VirtualBox* is chosen as the virtualization environment. *VirtualBox* is available for enterprise and home use and is freely available for both use-cases as Open Source Software under the terms of the GNU General Public License (GPL) version 2. The following chapter describes the setup of the then current version of *openSUSE* in a *VirtualBox* on your host operation system. *VirtualBox* is currently available for

➤ Windows ➤ OSX ➤ Linux ➤ Solaris

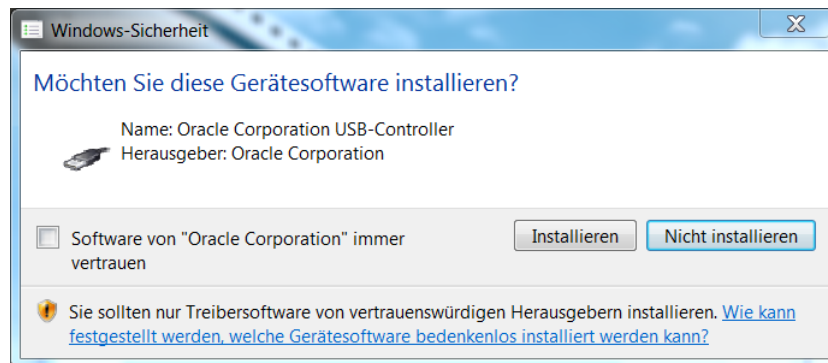
host operating systems. The current release of *VirtualBox* is available from:

<https://www.virtualbox.org/>

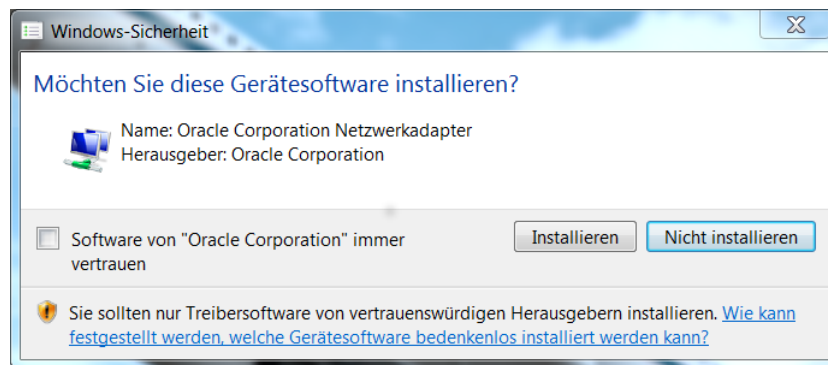
Go to the download section and choose the installer for your host operating system. The following description is valid for a Windows host and is tested for the 64bit variant of Windows 7. After the download execute the binary installer and follow the instructions of the setup wizard. In the custom setup step simply let all selected items enabled. Afterwards simply complete the wizard.



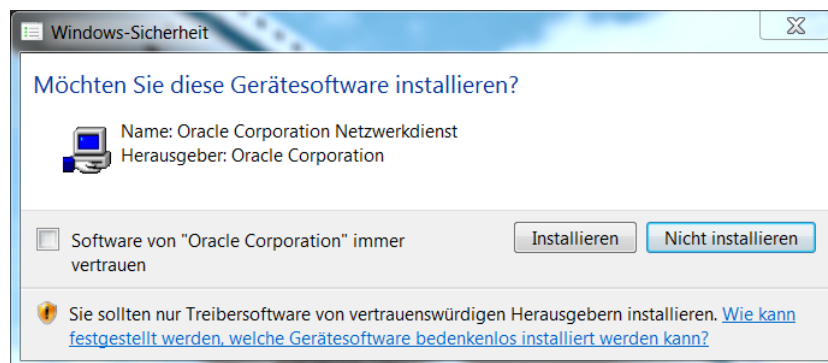
During the installation simply answer the following questions with *install* to allow access on the devices for the virtual machine.



(a) Install USB-Controller



(b) Install network adapter

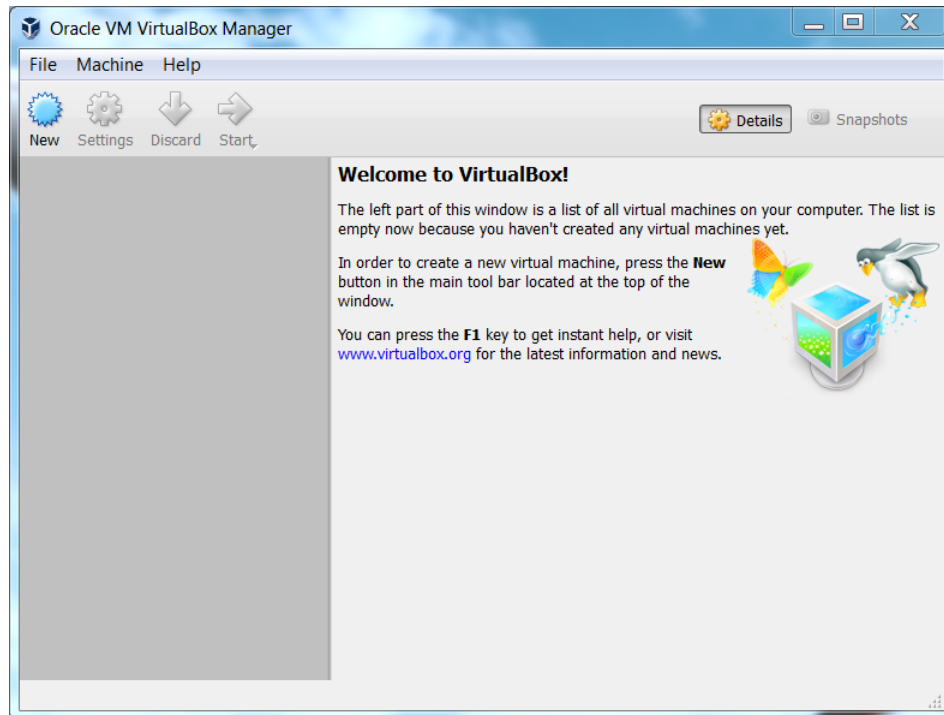


(c) Install network service

Figure 2.1.: Allow *VirtualBox* access to devices

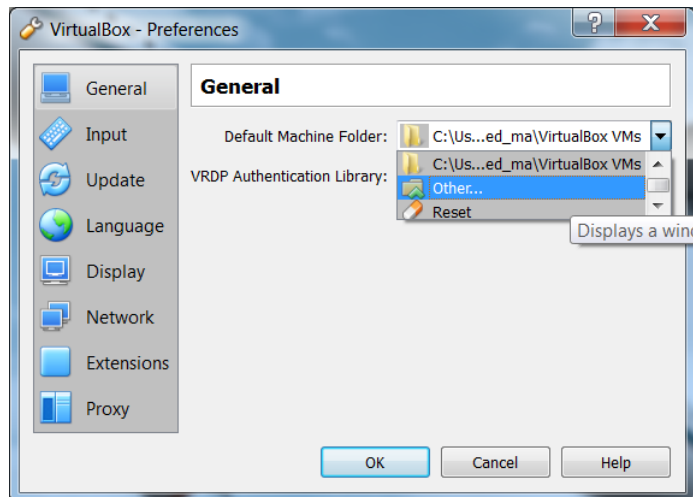
2.2.2. Create the virtual machine

After the installation is complete start the *VirtualBox* Manager.



Before we create a new virtual machine

- From the menu bar: Click *File*
- Click *Preferences*
- In the *General* tab select the *Default Machine Folder* to be a folder on a harddrive with sufficient amount of free memory to handle your virtual machine size, here 200GB

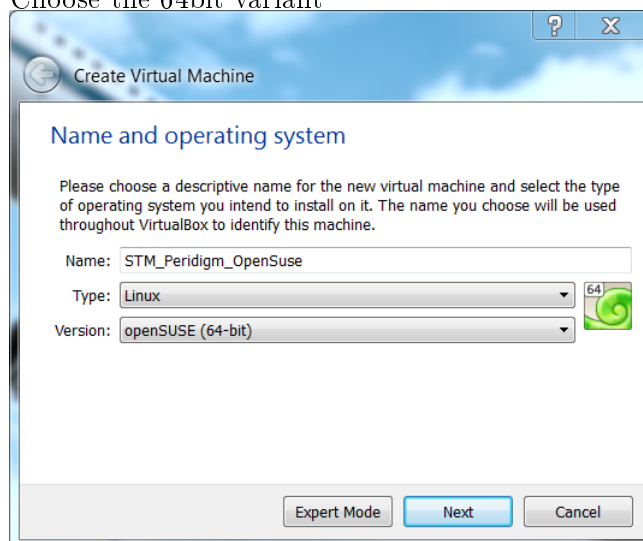


- Close the Preferences windows with a click in *Ok*

Now we can create a new virtual machine. Click *New* in the *VirtualBox* Manager main window. A dialog appears that guides you through the setup of the virtual machine.

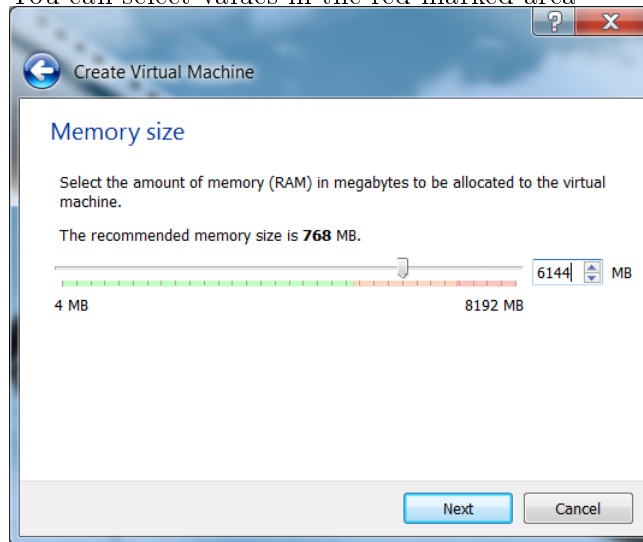
1. Select the virtual machine name, type and version

- Choose a name that includes the version & the selection automatically jumps to your choice
- Choose the 64bit variant



- A new folder with your chosen name is created in the directory you specified in the *General* tab of the *Preferences* toolbar menu
 - Click *Next*
2. Set the amount of RAM you grant your virtual machine
- The more RAM *Peridigm* has available the better

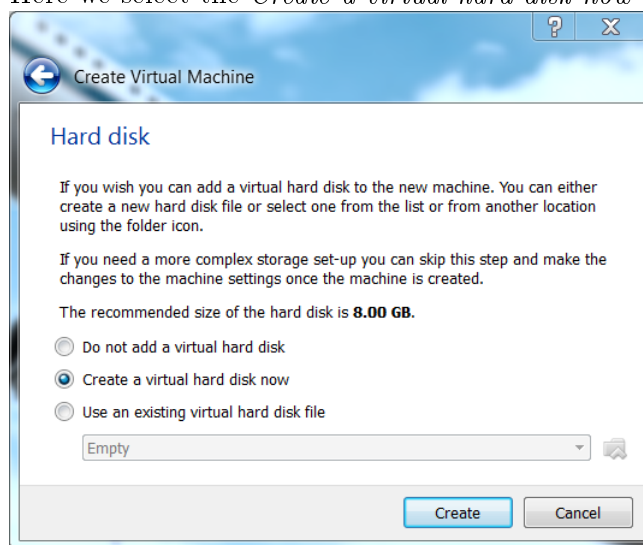
- But your host operating system also still needs some RAM left to work with
- Choose an integer multiple of 1024 as amount of RAM
- Leave the host operating system at least 2GB of RAM
- You can select values in the red marked area



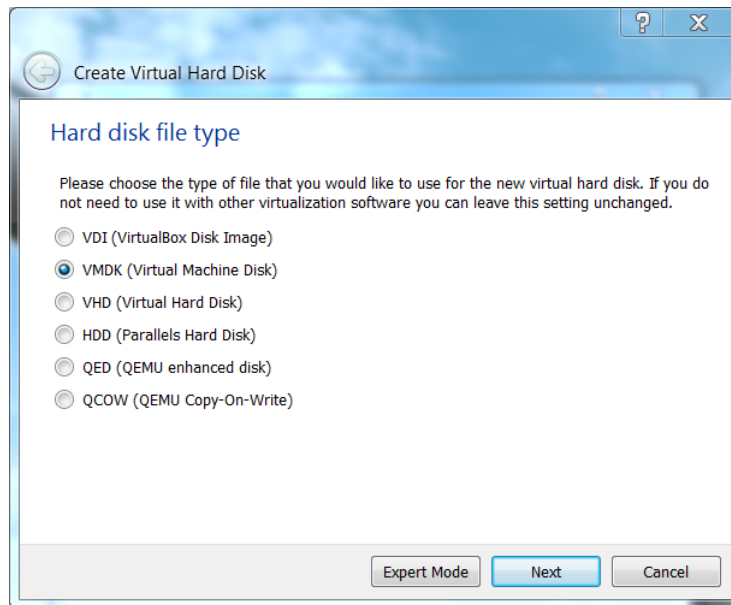
- Click *Next*

3. Create a virtual hard disk to install your distribution on

- Here we select the *Create a virtual hard disk now* option



- Click *Create*
- Select *VMDK (Virtual Machine Disk)* to allow use of this virtual hard disk in other virtualization tools like VMWare.

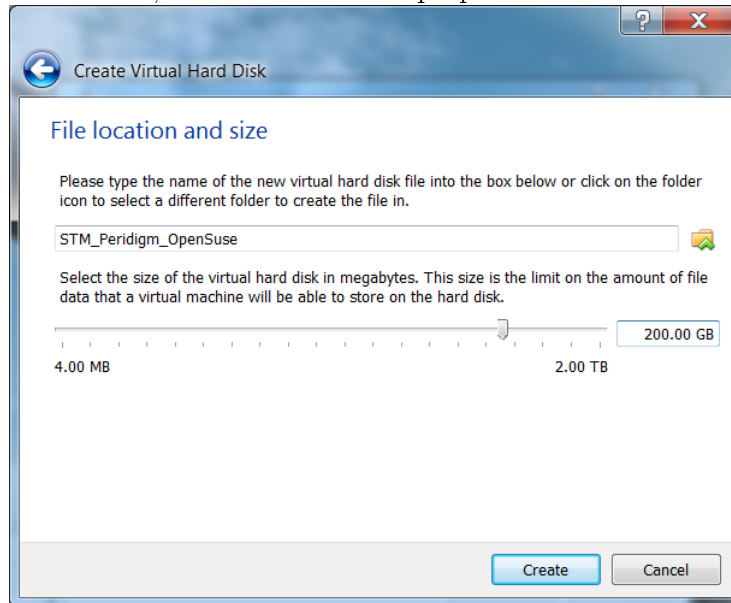


- Click *Next*
- Select *Fixed size*
- Do not select *Split into files less than 2GB*

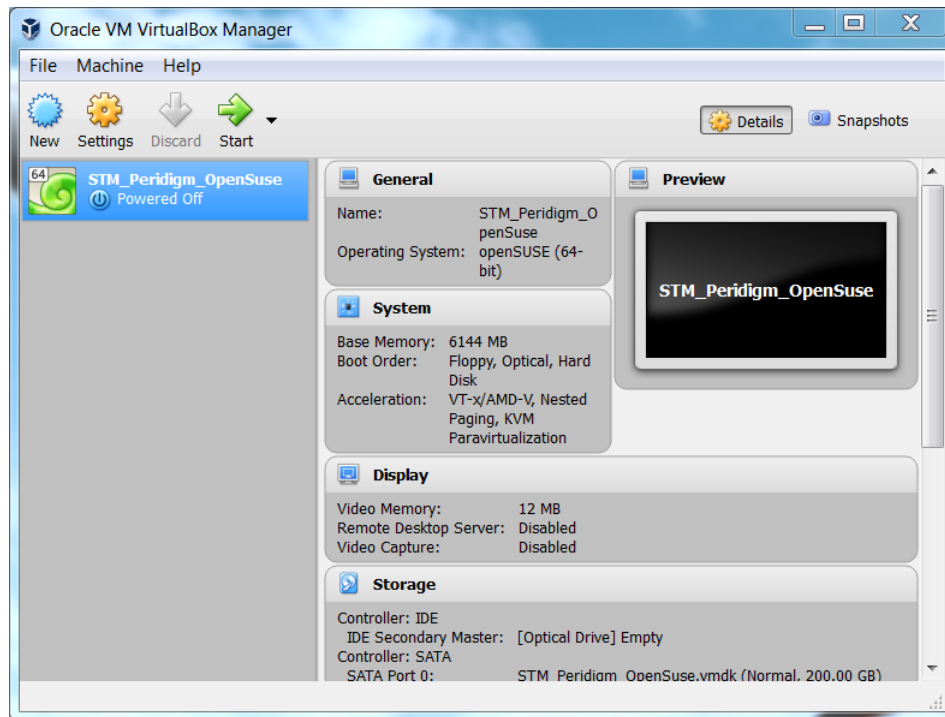


- Click *Next*
- Setup virtual hard disk name and size
- By default the name is identical to the virtual machine name
- If you click the folder button you can change the location of the virtual hard disk file. By default it is saved in your virtual machine folder in the directory specified in the *General* tab of the *Preferences* toolbar menu

- Set the size of the virtual hard disk to the amount you want and have free, here 200GB. Despite being saved in binary format, *Peridigm* result files can be quite big and for explicit time integration a lot of them are created. Despite a Linux distribution does not need nearly as much hard disk space as a Windows installation, at least 120GB are proposed as virtual hard disk size.

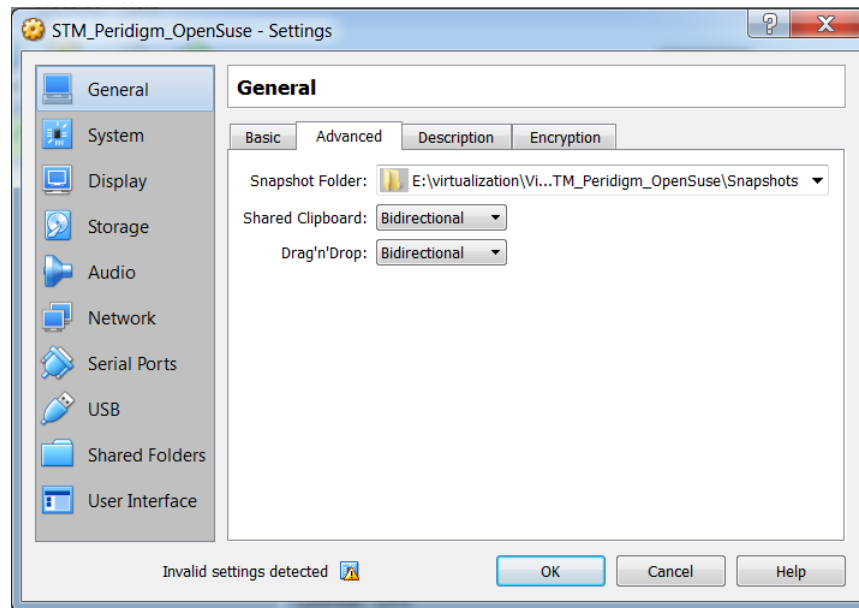


- Click *Create*
- Wait for the creation to finish
- Afterwards you have a new virtual machine

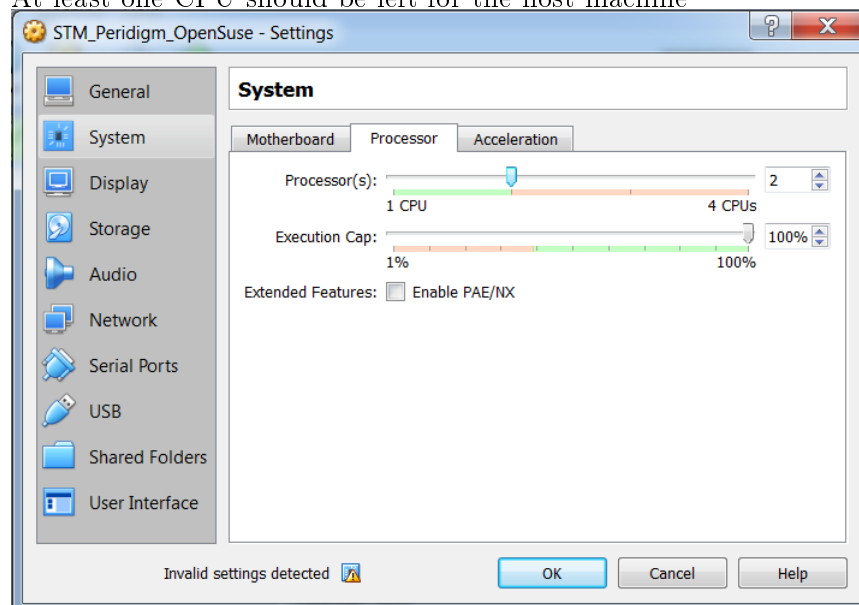


4. Before we install the Linux distribution inside the virtual machine, we have to configure some settings

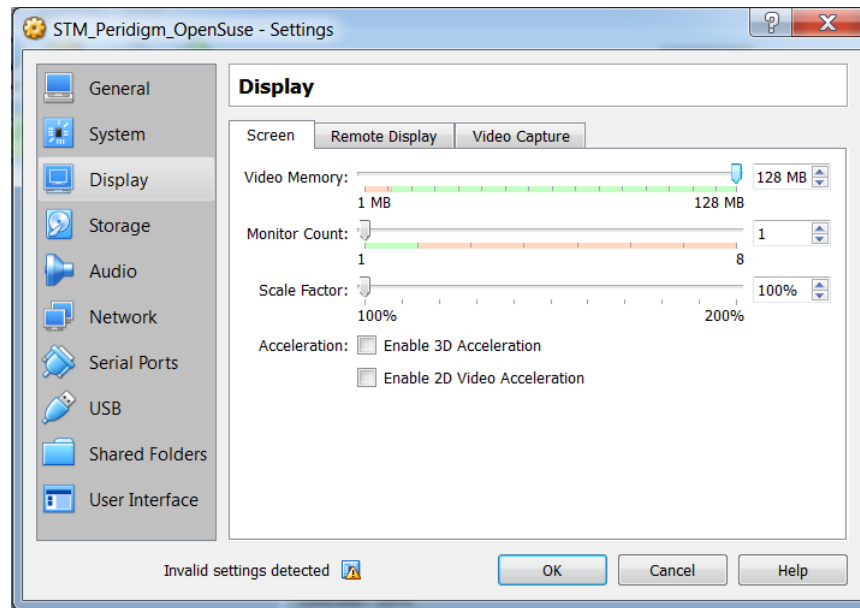
- Select the newly created virtual machine and click *Settings*
- In the *General* tab
 - Select *Advanced*
 - Select: *Shared Clipboard* Bidirectional
 - *Drag'n'Drop* Bidirectional



- Ignore the warning about *Invalid settings detected* if this is only a RAM issue
- In the *System* tab
 - Select *Processor*
 - Set *Processor(s)* to your preferred value
 - At least one CPU should be left for the host machine



- In the *Display* tab
 - Select *Screen*
 - Set *Video Memory* to maximum



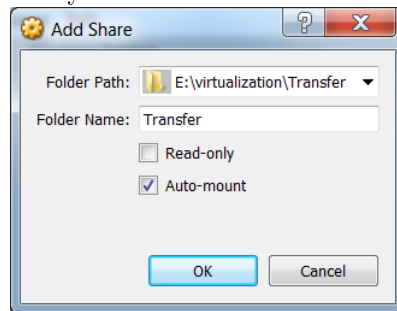
- Click *OK*

All modifications to the virtual machine preferences in step 4 can be modified after the installation of the virtual machine distribution in case the virtual machine is shut down.

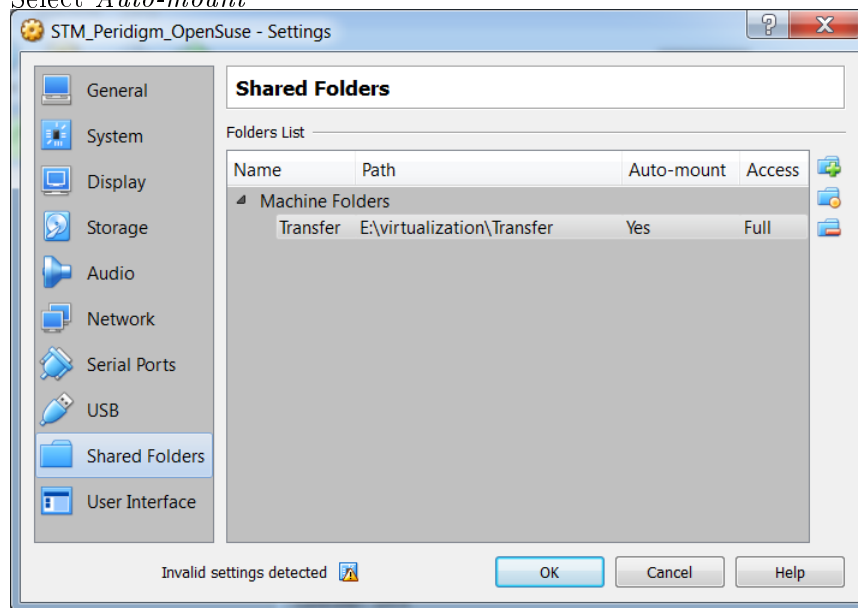
2.2.3. Create a shared folder between host and virtual machine

1. In the host operating system:
 - Open a Windows Explorer
 - Create a shared folder for the file exchange between the host and the virtual machine operating system anywhere it suits you or use an existing one, here the shared folder is `E:\virtualization\Transfer`
 - Right-Click the newly created folder and click *Properties*
 - In the *Shared Folders/Freigabe* tab
 - Click on *Freigabe*
 - In the dialog appearing click on the combobox arrow and select *Anyone/-Jeder*
 - Click *Freigabe*
 - Click *Close*
 - Be aware that the folder is visible in your whole network
2. Inside the virtual box manager:
 - Select the newly created virtual machine and click *Settings*
 - In the *Shared Folders* tab
 - Click the + folder button on the right

- In *Folder Path*: create or add a transfer folder between your host system and your virtual machine



- Select *Auto-mount*



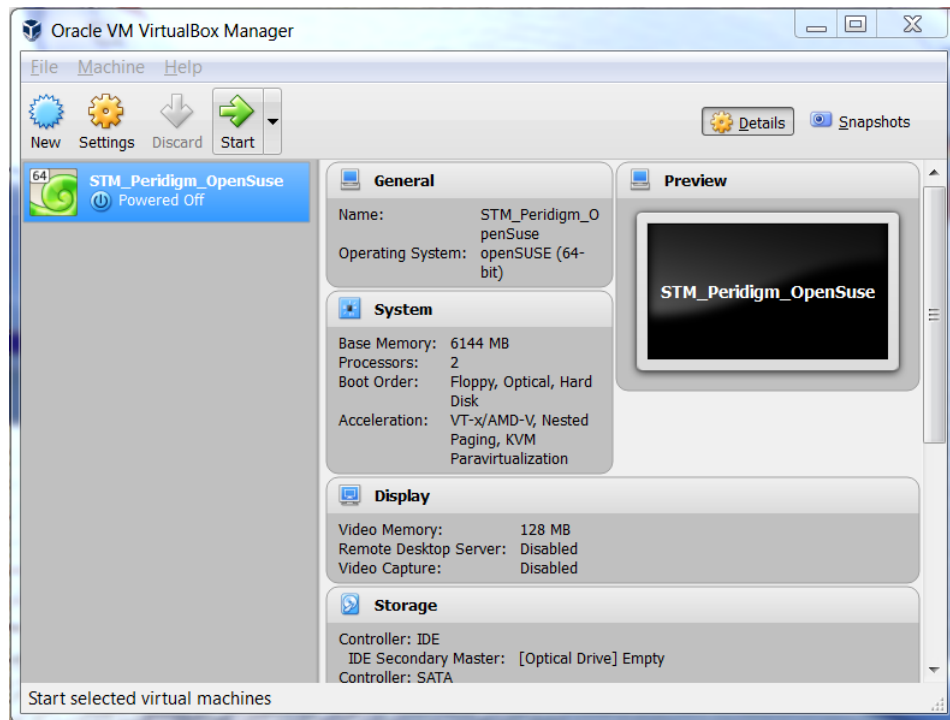
➤ Click *OK*

2.2.4. Install the operating system in the virtual machine

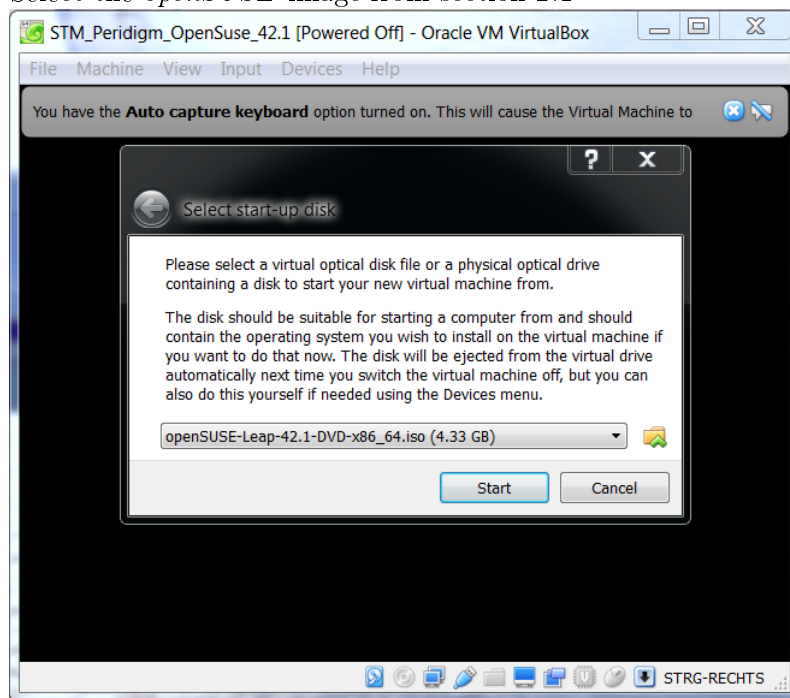
Now, we can install the virtual machine operating system:

1. Start the installation

➤ Select the virtual machine in the *VirtualBox* Manager and click *Start*



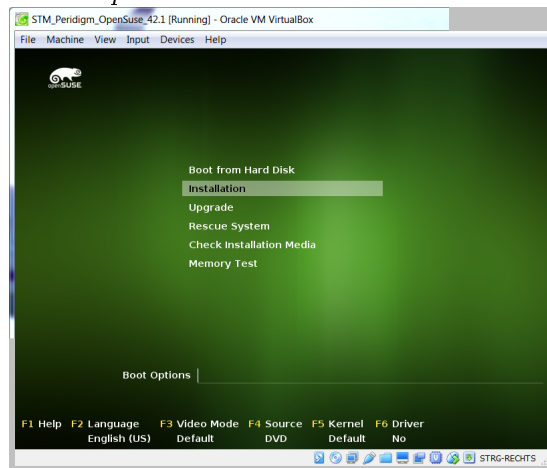
➤ Select the *openSUSE* image from section 2.1



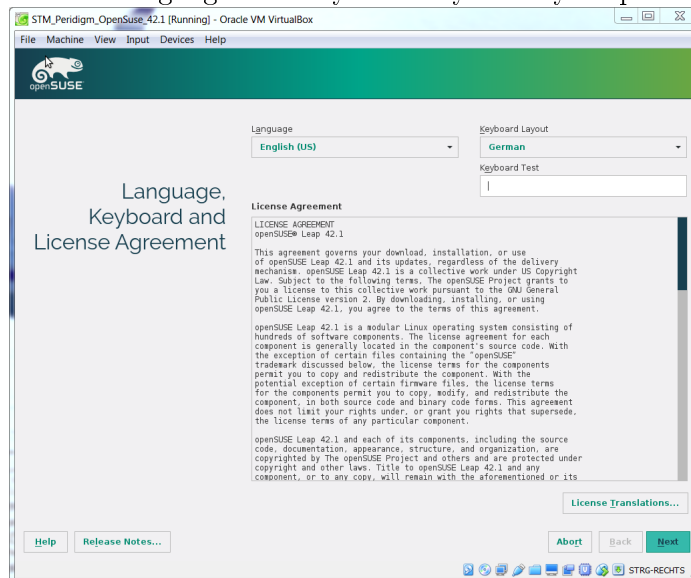
➤ Click *Start*

2. Setup the installation

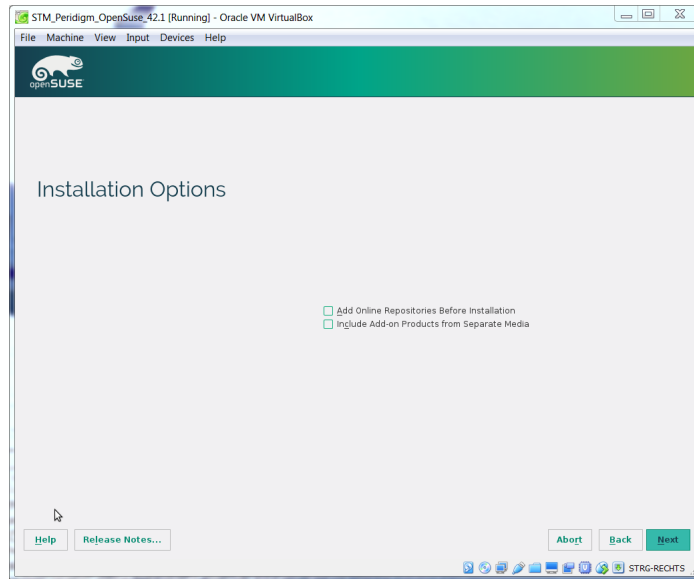
- In the *openSUSE* boot menu select *Installation*



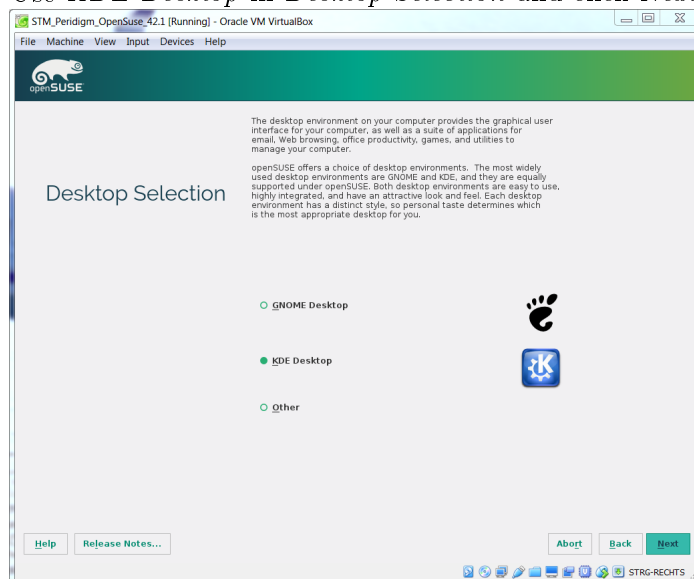
- Set the Language and Keyboard layout to your preferred option



- Click *Next*
- In the *Installation Options* to not toggle on any of the options

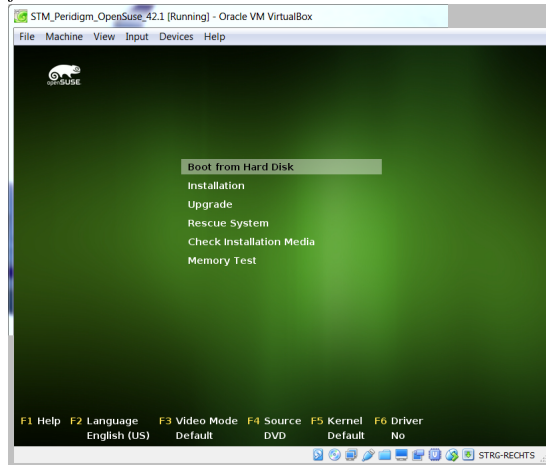


- Click *Next*
- Use the *Suggested Partition* and click *Next*
- Click on the Map to select your country to set *Clock and Time Zone* and click *Next*
- Use *KDE Desktop* in *Desktop Selection* and click *Next*

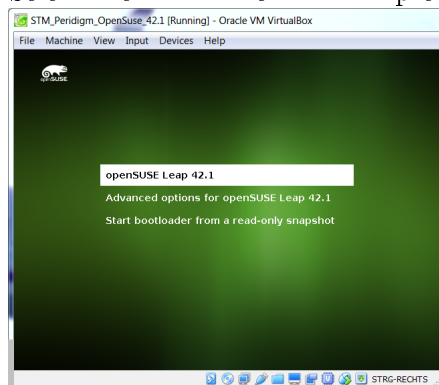


- Setup the first user name & password
 - You can use the same user and root password if you are and will always be the only user of your virtual machine
 - User: *Username* stm
Password 13112

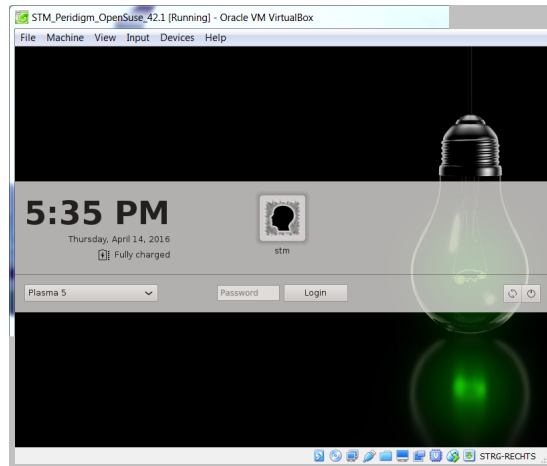
- Admin: *Password* dlr-fa-13112-bs
- Click next
- In the next windows click *Install*
- 3. After installation
- After the installation is complete virtual system restarts. Now select *Boot from Hard Disk*



- Select the normal version and press Enter



- Login with your password



- Open a shell
- Login as root user, perform

```
zypper refresh  
zypper update
```

And select yes to perform an operating system update

- Restart the virtual machine operating system

Ta-daa you have a linux installation inside of a virtual machine.

2.2.5. User modifications to use shared folders

In order for the Linux users to use the virtual machine shared folders

1. Open *YaST2*
2. In the *Security and Users* tab open User and Group Management
3. Select the user and click *Edit*
4. Go to *Details* tab
5. On the right select *users* and *vboxsf* as *Additional Groups* and click *OK*
6. Restart your virtual system

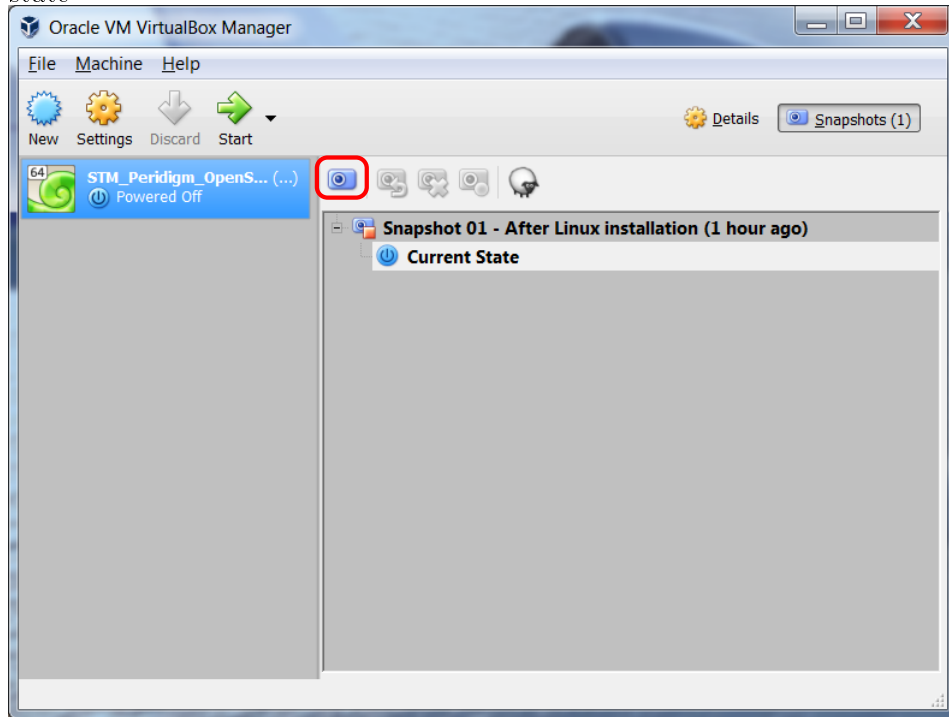
The shared folders are mounted under `/media/`. In the current case the single shared folder is accessible under `/media/sf_transfer/`.

2.2.6. Save the virtual machine state

After the operating system installation it is recommended to save a snapshot of the current virtual machine state. Thus, it is always possible to reset your virtual machine to this state in case anything goes wrong during the *Peridigm* installation.

To create a snapshot:

1. Open the *VirtualBox* Manager
2. In the upper right corner select *Snapshots*
3. Click the little camera button to take a snapshot of the current virtual machine state



3. *Peridigm* Linux installation

3.1. Tested combinations

3.1.1. CPU-Architecture & operating system

3.1.1.1. System 1 - STM-Laptop

Hardware:	CPU:	Name:	Intel Core i7 M620
		Architecture:	x86_64
		Cores:	4
		Threads:	4
		Clock rate:	2.67GHz
	RAM:	Amount:	8Gb
Software:	OS:	Name:	openSUSE
		Version:	42.1
		Type:	64bit

3.1.1.2. System 2 - Virtual machine

Hardware:	Host:	CPU:	Name:	Intel Core i7-4600U
			Architecture:	x86_64
			Cores:	2
			Threads:	4
			Clock rate:	2.1GHz
		RAM:	Amount:	8Gb
	VM:	CPU:	Cores:	2
		RAM:	Amount:	6Gb
Software:	Host:			VirtualBox 5.0
		VM: OS:	Name:	openSUSE
			Version:	42.1
			Type:	64bit

3.1.1.3. System 3 - STM-Cluster

Hardware:	CPU:	Name:	Intel Xeon E5-2407
		Architecture:	x86_64
		Number:	8
		Cores:	4
		Threads:	4
		Clock rate:	2.2GHz
	RAM:	Amount:	32Gb
Software:	OS:	Name:	SUSE Linux Enterprise Server
		Version:	11
		Patchlevel:	3
		Type:	64bit

3.1.2. Library and system combinations

Setup			1	2	3	4
System			STM-Laptop	VirtualBox	VirtualBox	STM-Cluster
Basics	Compiler	Fortran	gcc-fortran 4.8.5	gcc-fortran 4.8.5	gcc-fortran 4.8.5	gcc-fortran 4.8.5
		C	gcc 4.8.5	gcc 4.8.5	gcc 4.8.5	gcc 4.8.5
		C++	gcc-c++ 4.8.5	gcc-c++ 4.8.5	gcc-c++ 4.8.5	gcc-c++ 4.8.5
	<i>CMake</i>		3.4.3	3.4.3	3.5.1	3.5.2
	<i>MPI</i>	<i>Open MPI</i>	1.10.2	1.10.2	1.10.2	1.10.4
		<i>MPICH</i>	-	-	-	-
	<i>Python</i>		2.7.11	2.7.9	2.7.9	2.6.9
Libraries	<i>Boost</i>		1.55.0	1.55.0	1.60.0	?
	<i>HDF5</i>		1.8.16	1.8.16	1.10.0	?
	<i>NetCDF-C</i>		4.4.0	4.4.0	4.4.0	4.4.1
	<i>Trilinos</i>		12.4.2	12.4.2	12.6.1	?
	<i>Peridigm</i>		1.4.1	1.4.1	1.5.0	1.4.1

3.2. Basics

The following section describes the installation of the required basic packages for the *Peridigm* libraries. The subsections are in the order required for a proper installation.

3.2.1. Preliminary remarks

3.2.1.1. Installation shell

The following description is valid for an installation using the `bash` as shell. If you use any other shell, e.g. `ksh`, `csh` or their descendants you have to modify the environment variable parts of this guide or simply type `bash` and Enter in your `tcsh` to switch shells.

3.2.1.2. Download directories

During the course of this installation guide it will be necessary to download several source code packages. In the instructions the key `$DOWNLOAD_DIR` is the identifier for the download directory. The scripts in the appendix of this documents assume that

```
$DOWNLOAD_DIR=/usr/local/src/
```

You are free to choose any other folder as the download directory. If you do so, you have to modify the source code path in the scripts in the appendix accordingly.

3.2.1.3. PATH variable for user defined installation directories

It is assumed that the current installations are performed for all users of the device. Thus, the global installation directory `/usr/bin/` is used.

However, the installation directory for each tool can be changed, e.g. with

```
./configure --prefix="/home/$USER/TOOL"
```

If this is done, the path to the executables have to exported to the `PATH` variables.

```
export PATH="$PATH:/home/$USER/TOOL/bin"
export LD_LIBRARY_PATH="$LD_LIBRARY_PATH:/home/$USER/TOOL/lib/"
```

This has to performed for each individual installation directory.

NEVER EVER FORGET THE `$PATH:` AND `$LD_LIBRARY_PATH:` IN THE BEGINNING OR A NEW EMPTY PATH VARIABLE WILL BE CREATED AND ADDED TO. YOU WILL NOT BE ABLE TO USE ANYTHING USEFUL ON YOUR DEVICE BECAUSE ALL ALIASES WILL BE DELETED.

3.2.1.4. Installation user

All installations are performed as `root` user. To make sure that the end user is allowed to use the installed programs make sure that they have the necessary permissions. The default installation directory for installations with a package manager or *zypper* is `/usr/bin`. You can check if the permissions are correct by opening a terminal, navigation to `/usr/bin` and the command

```
ls -l | grep PARTOFTOOLABBREVIATION
```

For `ls -l | grep gcc` the result might look something like this:

```
lrwxrwxrwx 1 root root      7  5. Feb 14:07 cc -> gcc-4.8
lrwxrwxrwx 1 root root      7  5. Feb 14:07 gcc -> gcc-4.8
-rwxr-xr-x 1 root root 755680 29. Okt 18:02 gcc-4.8
lrwxrwxrwx 1 root root     10  5. Feb 14:07 gcc-ar -> gcc-ar-4.8
-rwxr-xr-x 1 root root  27136 29. Okt 18:02 gcc-ar-4.8
lrwxrwxrwx 1 root root     10  5. Feb 14:07 gcc-nm -> gcc-nm-4.8
-rwxr-xr-x 1 root root  27136 29. Okt 18:02 gcc-nm-4.8
lrwxrwxrwx 1 root root     14  5. Feb 14:07 gcc-ranlib -> gcc-ranlib-4.8
-rwxr-xr-x 1 root root  27144 29. Okt 18:02 gcc-ranlib-4.8
```

In the first column the current rights are specified. The first symbol shows if the current entry is a link or not. The nine symbol afterwards are the three individual rights for user, group and other. The three individual rights are r-read, w-write and x-execute.

If the permissions are not set correctly, consult the documentation of *chmod*.

3.2.2. Root .bashrc file

You usually login as a normal user to *openSUSE* but changes to the system are performed as root user.

During this installation guide modifications of the `.bashrc`, a hidden file in the user home directory are requested. For the installation process as root user it is necessary that these modifications also take effect for the root user.

To achieve this a symbolic link is created in the root home directory to the modified `.bashrc` in the ordinary user directory. To achieve this open a console and perform the following steps

```
su                # Switch to root user
cd                # Change to root home
ln -sf /home/$USERNAME/.bashrc .  # Create symbolic link
```

This way, the root `.bashrc` file is always an identical copy of the one of the user with the name `$USERNAME` here.

3.2.3. Fortran & C & C++-compiler

Peridigm as well as *Python* python require an acceptable C or C++-compiler. *Trilinos* additionally needs a Fortran-compiler. Here, the free *GNU Compiler Collection* versions, short *GCC* are used. The current release and further informations can be found on

<https://gcc.gnu.org/>

Currently, there are two main versions available, *GCC*, which is basically *GCC* version 4.8, as well as *GCC5*. The installation of the used *Python* currently seems not to work with *GCC5*. Additionally, *Trilinos* needs a compiler that is **C++11** compliant and thus needs *GCC* version **4.7.2 or later**. Therefore *GCC* version 4.8 is used. If using Intel compilers, version 13 or later is required by *Trilinos*.

Normally, the *GCC* repository is already part of an *openSUSE* distribution. To check the availability of the *GCC*-repository in your *openSUSE* distribution open a terminal as root and use the following command to get a list of all repositories.

```
zypper repos
```

Installation with *YaST2*

To install the Fortran-, C- and C++-compilers of *GCC* with the package manager perform the following steps:

1. Open *YaST2*
2. Click on *Install software*
3. Go to the *Search* tab
4. Search for *GCC*
5. Check *gcc-fortran*, *gcc* and *gcc-c++*
6. Click on apply

Installation from source

ToDo

Installation with *openSUSE*-repository

To use *zypper* open a terminal as root. Use the following commands to install Fortran-, C- and C++-compilers of *GCC* from the repositories. Answer the questions if installation shall continue with yes.

```
zypper install gcc-fortran
zypper install gcc
zypper install gcc-c++
```

The installation usually is performed to `/usr/bin/`. If another installation directory is used, it has to be made sure, that this directory is part of the `$PATH`-variable. To check if this is the case, open a terminal type

```
echo $PATH
```

The installation directory has to be an entry of the printed string.

3.2.4. *CMake*

CMake is cross-platform free and open-source software for managing the build process of software using a compiler-independent method. It is maintained by Kitware. The official homepage of is *CMake*

<https://cmake.org/>

Trilinos release 12.4 and higher use a *CMake* build system, which requires *CMake* version **2.8.11 or newer**.

Installation from source

In order to install *CMake* from the official or any other binary source open a terminal and login as root. Change directory to the designated download folder, e.g. `/usr/local/src/` and perform the following steps:

```
cd $DOWNLOAD_DIR
wget http://www.cmake.org/files/v3.4/cmake-3.4.3.tar.gz # Download
tar xvfz cmake-3.4.3.tar.gz                          # unzip
cd cmake-3.4.3                                         # go into directory
./configure --prefix=/usr/local/bin/cmake-3.4.3 > configure_cmake.log 2>&1
make > make_cmake.log 2>&1                             # build
make install > make_install_cmake.log 2>&1            # install
```

If you want to see the available configuration options, run the command below in the terminal.

```
./configure --help
```

In order to configure the installation directory of *CMake* before installation, run the command below

```
./configure --prefix=/opt/cmake
```

After installation without any errors you can verify the installation by running the command below:

```
/usr/local/bin/cmake-3.4.3/bin/cmake -version
```

The output should look something like below (depending upon *CMake* version you are installing).

```
cmake version 3.4.3
```

Afterwards, the *CMake*-directory has to be added to the `PATH` environment variable

```
export PATH=$PATH:/usr/local/bin/cmake-3.4.3/bin
```

Installation with *openSUSE*-repository

For the installation of the build process manager *zypper* visit:

<http://software.opensuse.org/download.html?project=server%3Airc&package=cmake>

You can either choose the 1-Click-installation or add the repository and install manually. For the latter login to a terminal as `root` and type

```
zypper addrepo http://download.opensuse.org/repositories/server:irc/  
    openSUSE_Leap_42.1/server:irc.repo  
zypper refresh  
zypper install cmake
```

3.2.5. MPI

For parallel computations on multiple cores an implementation of the Message Passing Interface is required. Only **one** of the the following possibilities is required. The current implementation uses *Open MPI*.

3.2.5.1. *Open MPI*

Open MPI is an open source Message Passing Interface implementation that is developed and maintained by a consortium of academic, research, and industry partners. The current version and further information can be found at

<https://www.open-mpi.org>

Installation with *YaST2*

To install *Open MPI* with the package manager perform the following steps:

1. Open *YaST2*
2. Click on *Install software*
3. Go to the *Search* tab
4. Search for Open MPI
5. Check Open MPI
6. Click on apply

Installation with *openSUSE*-repository

The *Open MPI*-repository is part of the openSUSE distribution. Therefore, it can be directly installed from the system repositories.

To use *zypper* open a terminal as root. Use the following commands to install *Open MPI* from the repositories. Answer the questions if installation shall continue with yes.

```
zypper install openmpi
```

Installation from source

The Gzipped tarball source files can be obtained from

<https://www.open-mpi.org/software/ompi/>

In the subfolder choose the version of your liking. Change directory to the designated download folder, e.g. `/usr/local/src/` and perform the following steps:

```
cd $DOWNLOAD_DIR
wget https://www.open-mpi.org/software/ompi/v1.10/downloads/openmpi-1.10.2.tar.gz
tar xvfz openmpi-1.10.2.tar.gz          # unzip
cd openmpi-1.10.2                      # go into directory
./configure --prefix=/usr/local/lib/openmpi-1.10.2 > configure_openmpi.log 2>&1
make > make_openmpi.log 2>&1           # build
make altinstall > make_install_openmpi.log 2>&1
```

If no previous version of *Open MPI* exists use `make install` instead of `make altinstall`.

Set the PATH variables

Unfortunately the *Open MPI* installation does not work out of the box. You need to set the `PATH` and `LD_LIBRARY_PATH` variables and edit a configuration file first.

The `LD_LIBRARY_PATH` must be set so that *mpi4py* can find the *Open MPI* libraries.

In bash do for 32-bit

```
export PATH=$PATH:/usr/local/lib/openmpi-1.10.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/openmpi-1.10.2/lib
```

or 64-bit

```
export PATH=$PATH:/usr/local/lib/openmpi-1.10.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/openmpi-1.10.2/lib64
```

We recommend you add this line to your `.bashrc` file in case you use *Bash* or call `setenv` and edit the `.cshrc` file if you use a C shell so that the variable is set correctly for all sessions. For the modification of user `.bashrc` file for all libraries, please consult section A.7.

3.2.5.2. MPICH

MPICH is a high performance and widely portable implementation of the Message Passing Interface (MPI) standard.

Use the operating system distribution

ToDo

Use 1-click install

Go to

<https://software.opensuse.org/package/mpich>

and choose 1-Click-Install or download the rpm-file from the source.

Installation with *openSUSE*-repository

ToDo

Installation from source

Try

```
cd $DOWNLOAD_DIR
zypper si -d mpich2                                # install the build deps
                                                    # for the previous version
wget http://www.mpich.org/static/downloads/3.2/mpich-3.2.tar.gz
tar xvfz mpich-3.2.tar.gz                          # unzip
cd mpich-3.2                                        # go into directory
./configure > configure_mpich.log 2>&1
make > make_mpich.log 2>&1                          # build
make altinstall > make_install_mpich.log 2>&1      # install
```

3.2.6. *Python*

Use the operating system distribution

Python is already part of an openSUSE standard installation since also system components require python. The installed version can be shown in the terminal by the command

```
python -V
```

Packages are available for both *Python* 2.7 as well as *Python* 3.x. A parallel installation if *Python* 2 and *Python* 3 possible without problems or package conflicts.

To update the python distribution to the newest available state in the OS repositories, open a terminal, login as **root**\verb and use the following command

```
zypper update python
```


Additionally, `python-devel` is required, so

```
zypper install python-devel
```

Perform a new installation

If no initial version of *Python* is present in the operating system it is necessary to download the source and install the source. For the latest or required version of *Python* visit

<http://www.python.org/download/>

For the installation, open a terminal and change directory to `/home/USERNAME/bin` for a single-user installation or `/usr/local/bin` for an installation for all users

```
cd $DOWNLOAD_DIR
wget https://www.python.org/ftp/python/2.7.11/Python-2.7.11.tgz # Download
tar xvfz Python-2.7.11.tgz # unzip
cd Python-2.7.11 # go into directory
./configure
make # build
make altinstall # install
```

Afterwards, you are free to delete the downloaded Gzipped source tarball, here

```
cd $DOWNLOAD_DIR
rm Python-2.7.11.tgz # delete
```

3.3. System libraries

3.3.1. Necessary libraries

Install or update the following system libraries in advance of the *Peridigm* library installation.

```
zypper install libbz2-devel
zypper install zlib-devel

zypper install m4

zypper install blas
zypper install lapack
zypper install libX11-devel
```

3.3.2. Libraries that are not supposed to be installed yet

Open *YaST2* and go to *Software Management*. In the *Search* field type *HDF5* and look whether an older version than the *HDF5* version you want to use is already installed on the system.

This is the case if you have *octave-forge-netcdf* installed on your system. If you do not really use this package you can uninstall it in *YaST2* together with the installed *HDF5* libraries.

If you really need *octave-forge-netcdf* which comes with *HDF5*-1.8.15 and have it installed already you can skip the installation of *HDF5* described here and change the rest of the installation to use version 1.8.15 of *HDF5*.

3.4. Libraries

3.4.1. *Boost*

Boost provides free peer-reviewed portable C++ source libraries. *Boost* libraries are intended to be widely useful, and usable across a broad spectrum of applications. For more informations and the current release visit

<http://www.boost.org/>

Peridigm requires *Boost*, version **1.37 or later**, including the *regex* and *unit_test* compiled libraries. *Boost* installations on many systems include header files only. This is not sufficient, the required libraries must be compiled and installed. To ensure proper execution of *Peridigm* and its unit tests, add the *Boost* directory `$INSTALL_DIR/lib` to your `LD_LIBRARY_PATH` (Linux) and/or `DYLD_LIBRARY_PATH` (Mac) environment variables.

Use 1-click install

There is a *RPM Package Manager* file available on the *openSUSE* homepage. However, *Boost* requires some additional libraries to be compiled specifically. Therefore, it is not tested if the following installation with the 1-click install option is sufficient for *Peridigm*. It is recommended to use the installation using the source files from a Gzipped tarball as described in the next paragraph.

Go to

<https://software.opensuse.org/package/boost>

and choose 1-Click-Install or download the rpm-file from the source. Be cautious, the version offered is not necessarily up to date. Consult

<http://www.boost.org/>

for the current release.

Installation from source

The current release of *Boost* is available from

<http://www.boost.org/>

and sourceforge:

<http://sourceforge.net/projects/boost/files/boost/>

Originally, I tried to install the then-current version 1.60. Unfortunately, this led to compilation errors in combination with the current version of the *GCC*-compiler. After searching for a solution of the issue, version 1.55 is recommended.

First, the additional libraries *libbz2-devel* and *zlib1g-dev* have to be installed in section 3.3 before we can install *Boost*. Additionally a new root shell must be opened to load the new environment variable additions for *Open MPI*.

```
cd $DOWNLOAD_DIR
wget http://sourceforge.net/projects/boost/files/boost/1.55.0/
    boost_1_55_0.tar.gz
tar xvfz boost_1_55_0.tar.gz          # unzip
cd boost_1_55_0                      # go into directory
```

Afterwards, create the *Boost* build script as described in section A.1. In order to use the script make it executable as described in section A.6. Open a terminal as root, change directory to the created install script and execute it with

```
./install_boost-1.55.0.sh > install_boost.log 2>&1
```

The printout of the installation is written to *install.log*. It should be checked if all components of *Boost* are compiled correctly.

Afterwards, the *Boost*-directory has to be added to the *LD_LIBRARY_PATH* environment variable

```
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/boost-1.55.0/lib
```

3.4.2. *HDF5*

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data. For further information visit

<https://www.hdfgroup.org/HDF5/>

HDF5 version **1.8.9 or newer** is required by *NetCDF-C* and the *SEACAS Trilinos* package. *HDF5* should be configured with the `--enable-parallel` option.

Installation with *openSUSE*-repository

HDF5 is available in an *openSUSE*-repository and can be installed using *zypper*. However, it is recommended to use the manual install with the Gzipped tarball to make sure the correct options are set.

```
zypper addrepo http://download.opensuse.org/repositories/home:ocefpaf/  
    openSUSE_Tumbleweed/home:ocefpaf.repo  
zypper refresh  
zypper install hdf5
```

Installation from source

The *HDF5* source code is available from

<https://www.hdfgroup.org/HDF5/>

Download the source code for your platform

```
cd $DOWNLOAD_DIR  
wget http://www.hdfgroup.org/ftp/HDF5/current/src/hdf5-1.8.16.tar.gz  
tar xvfz hdf5-1.8.16.tar.gz          # unzip  
cd hdf5-1.8.16                      # go into directory
```

Afterwards, create the *HDF5* build script as described in section A.2. In order to use the script make it executable as described in section A.6. Open a terminal as root, change directory to the created install script and execute it with

```
./install_hdf.sh > install.log 2>&1
```

Afterwards, the *HDF5*-directory has to be added to the `PATH` and `LD_LIBRARY_PATH` environment variable

```
export PATH=$PATH:/usr/local/bin/hdf5-1.8.16/bin  
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/hdf5-1.8.16/lib64
```

3.4.3. NetCDF-C

NetCDF-C (Network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. Distributions are provided for Java and C/C++/Fortran. For more information visit

<http://www.unidata.ucar.edu/software/netcdf/>

NetCDF-C is required by the *Trilinos SEACAS* package. *NetCDF-C* should be configured with the `--disable-netcdf-4` and `--disable-dap` options.

Installation from source

The *NetCDF-C* source code is available from the *NetCDF-C* homepage. Download the source code for your platform

```
cd $DOWNLOAD_DIR
wget ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf-4.4.0.tar.gz
tar xvfz netcdf-4.4.0.tar.gz          # unzip
cd netcdf-4.4.0                      # go into directory
```

Prior to compiling *NetCDF-C*, it is recommended that you modify the file `netcdf.h` in `$DOWNLOAD_DIR/netcdf-4.4.0/include/` to better support large-scale *Peridigm* simulations. Modify the following `#define` statements in the `netcdf.h` file. Change the values to match what is given below.

```
#define NC_MAX_DIMS      65536
#define NC_MAX_ATTRS     8192
#define NC_MAX_VARS      524288
#define NC_MAX_NAME      256
#define NC_MAX_VAR_DIMS  8
```

Afterwards, create the *NetCDF-C* build script as described in section A.3. In order to use the script make it executable as described in section A.6. Open a terminal as root, change directory to the created install script and execute it with

```
./install_netcdf.sh > install.log 2>&1
```

Due to an apparent glitch in the *NetCDF-C* installer, in some cases it may be necessary to manually copy the file `$DOWNLOAD_DIR/netcdf-4.4.0/include/netcdf_par.h` from the source distribution into the installation include subdirectory.

```
cp $DOWNLOAD_DIR/netcdf-4.4.0/include/netcdf_par.h /usr/local/bin/netcdf
-4.4.0/include/
```

Afterwards, the *NetCDF-C*-directory has to be added to the `PATH` and `LD_LIBRARY_PATH` environment variable

```
export PATH=$PATH:/usr/local/bin/netcdf-4.4.0/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/netcdf-4.4.0/lib64
```

3.4.4. *Trilinos*

The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages. For more information visit

<https://trilinos.org/>

A number of *Trilinos* packages are required by *Peridigm*. The *Trilinos* source code distribution includes the full set of *Trilinos* packages, each of which may be activated or deactivated using *CMake* build options, as described below. It is recommended that Makefiles be created by running **cmake** from the command line, as opposed to using the **ccmake** GUI.

The current release of *Trilinos* can be obtained from the download section of the *Trilinos* homepage. The download needs a short registration with a valid email-address. The download link is likely to be not reachable without the registration.

```
cd $DOWNLOAD_DIR
wget http://trilinos.csbsju.edu/download/files/trilinos-12.4.2-Source.tar
.gz
tar xvfz trilinos-12.4.2-Source.tar.gz
```

Trilinos does not allow the use of the directory with the source-files for the further progress of the installation. Therefore, create a new folder

```
mkdir trilinos-12.4.2
```

and copy the file from section A.4 to the new folder. Change the line for the *Open MPI*- and the *Trilinos*-source-directory (last line) if necessary.

In order to use the script make it executable as described in section A.6. Open a terminal as root, change directory to the created path and execute it with

```
./cmake_trilinos.cmake > cmakeopts.log 2>&1
```

Once *Trilinos* has been successfully configured, it can be compiled and installed as follows:

```
make -j 4
```

If there occur any errors during the compilation of *Trilinos* visit section B. For compiling with **make -j 4** more than 8GB of RAM are necessary. If you do not know if there were any compilation errors have occurred due to the long duration of the compilation process, repeat

```
make
```

after the original compilation with **make -j 4**. Only failed compilations are repeated. Afterwards perform

```
make install
```

The final installation can be found in the folder specified in `CMAKE_INSTALL_PREFIX:PATH` in the script from section A.4.

Afterwards, *Trilinos* has to be added to the `PATH` and `LD_LIBRARY_PATH` environment variables to later use the *Trilinos* decomposition features for the model decomposition for calculation on multiple processors.

```
export PATH=$PATH:/usr/local/bin/trilinos-12.4.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/trilinos-12.4.2/
lib
```


3.5. *Peridigm*

3.5.1. Download

3.5.1.1. Download the official release

The current official release of *Peridigm* can be obtained from the download section of <https://peridigm.sandia.gov/>

The download needs a short registration with a valid email-address. Download the `tgz` file of your preferred *Peridigm* version to `$DOWNLOAD_DIR`. Unpack the archive:

```
cd $DOWNLOAD_DIR
tar xvfz Peridigm_1.4.1.tgz
```

3.5.1.2. Download the latest master version from *GitHub*

The *Peridigm* repository is available from *GitHub* and can be downloaded from:

<https://github.com/peridigm/peridigm>

To obtain the latest master release go to that homepage and select the *master* branch in the top left and click on *Download zip* in the top right corner as shown by the red rectangles in Figure 3.1 or click this [link](#).

Unpack the archive:

```
cd $DOWNLOAD_DIR
unzip peridigm-master.zip
mv peridigm-master Peridigm-1.4.1-Source
```

3.5.1.3. Checkout the latest version from *GitHub*

With `svn`

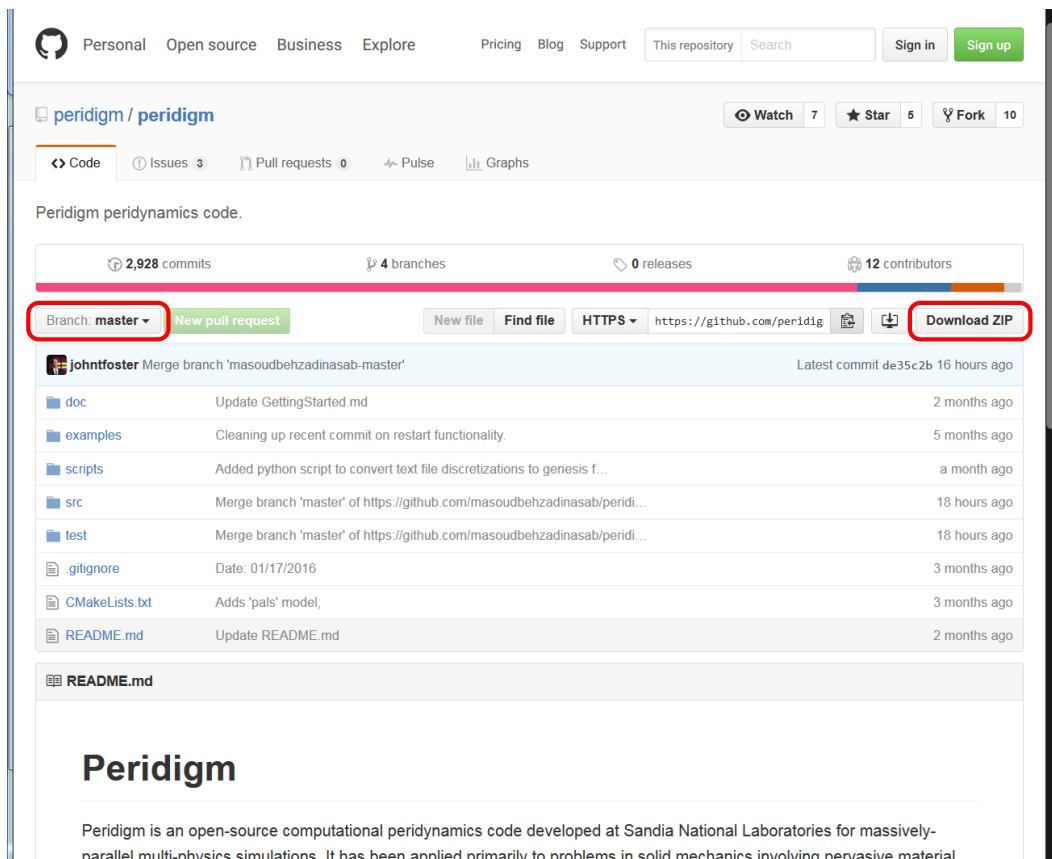
Use *kdesvn* to checkout the latest version. Checkout

<https://github.com/peridigm/peridigm.git/trunk>

With `git`

Use *git* on the cluster:

```
git clone https://github.com/peridigm/peridigm.git
```

Figure 3.1.: *Peridigm* GitHub repository screenshot

3.5.2. Compiling & installation

Peridigm utilizes the *CMake* build system. It is recommended that Makefiles be created by running `cmake` from the command line, as opposed to using the `ccmake` GUI.

The installation here is described for the then official *Peridigm* version 1.4.1. The steps for version 1.5 are identical besides the changes in folder names.

Peridigm does not allow the use of the directory with the source-files for the further progress of the installation. Therefore, create a new folder

```
mkdir Peridigm-1.4.1
```

and copy the file from section A.5 to the new folder. Change the lines for the library paths and the *Peridigm*-source-directory (last line) if necessary.

In order to use the script make it executable as described in section A.6. Open a terminal as root, change directory to the created path and execute it with

```
./cmake_peridigm.cmake > cmakeopts.log 2>&1
```

Once *Peridigm* has been successfully configured, it can be compiled and installed as follows:

```
make -j 4  
make install
```

The default location for the created binary is `/usr/local/bin/`. In case you want to create the binary at a different location add the following line to the script from section A.5

```
-D CMAKE_INSTALL_PREFIX=/PATH/TO/DESTINATION
```

After installation make sure to change permissions of the installation directory for the necessary users and groups.

3.5.3. After building and installing

[2] recommends to run `ctest` in your build directory after building and installing *Peridigm* to run all tests and confirm that you have a clean build. Alternatively, *Peridigm* offers an own test suite which is used here.

To be able to execute the test you first have to temporarily change the source and installation folder owner. Thus perform the following commands before executing the test.

```
chown -R $USERNAME:$GROUPNAME Peridigm-1.4.1  
chown -R $USERNAME:$GROUPNAME Peridigm-1.4.1-Source
```

Before starting the test-suite as a normal user, open a new shell or use an existing one and re-register your username to load the current state of the `.bashrc`-file:

```
su - $USERNAME
```

The *Peridigm* test suite is then run from the terminal as non-root user as follows:

```
make test
```

Remember to revert the modifications to the *Peridigm* directory ownership after it is assured that all tests are passed with:

```
chown -R root:root Peridigm-1.4.1  
chown -R root:root Peridigm-1.4.1-Source
```

3.5.4. Install a local version on the cluster

1. Login to the STM cluster and move to a directory of your convenience
2. Clone your local *Peridigm* version from GitHub with `git clone` or download the master zip-file and unpack, see section 3.5.1.1
3. Allocate cluster-node exclusively for building

```
salloc --exclusive
```

4. Load build and library environment

```
. /cluster/software/slurm/etc/env.d/mpibuild.sh  
. /cluster/software/slurm/etc/env.d/peridigm.sh
```

5. Change directory to the folder, where the unpacked *Peridigm* source folder is located

```
cd ~/src/peridigm
```

6. Create a build-directory and go to the new directory

```
mkdir peridigm-build  
cd peridigm-build
```

7. Save the following lines in the file `cmake_peridigm.cmake`. Change the path in the code to the correct location.

```
cmake \  
-D CMAKE_BUILD_TYPE:STRING=Release \  
-D CMAKE_INSTALL_PREFIX=/home/USER/peridigm-build \  
-D CMAKE_CXX_FLAGS:STRING='-O2 -Wall -std=c++11 -pedantic -Wno-long-  
long -ftrapv -Wno-deprecated' \  
/home/USER/peridigm-master
```

8. Call CMake via terminal with the given code:

```
./cmake_peridigm.cmake
```

9. Make

```
make -j 8
```

10. Test

```
make test
```

11. Create the executable

```
make install
```

12. Exit salloc shell

```
exit
```

13. The executable is now located at `~/src/peridigm/peridigm-build/bin`

14. For how to execute the local version using the cluster queuing-system look at the Peridigm User Guide

A complete script for cloning Peridigm from GitHub, compiling and installing on the cluster can be found in subsection A.5.2.

3.5.5. Use of *Docker*

<http://johnfoster.github.io/posts/peridigm-without-building-via-Docker.html>

4. Running *Peridigm*

A dedicated description on how to run *Peridigm* can be found in the *Peridigm* Users Guide which is part of the same repository as this document.

5. Install *ParaView*

ParaView is an open source multiple-platform application for interactive, scientific visualization. The current release and further informations can be found on

<http://www.paraview.org/>

ParaView was developed to analyze extremely large datasets using distributed memory computing resources.

5.1. Linux installation

Use 1-click install

Go to

<https://software.opensuse.org/download/package?project=science&package=paraview>

and choose 1-Click-Install or download the rpm-file from the source.

Installation with *openSUSE*-repository

ParaView is part of the *openSUSE* Science Repository. The repository can be included into the package management.

```
zypper addrepo http://download.opensuse.org/repositories/science/  
    openSUSE_Leap_42.1/science.repo  
zypper refresh  
zypper install paraview
```

Installation from source

The source code of the current *ParaView* release is available from the download section of the *ParaView* homepage. For an installation using the source code and *CMake* please consult

http://www.paraview.org/Wiki/ParaView:Build_And_Install

5.2. Windows installation

Go to the download section of the *ParaView* homepage and download the binary installers for your windows operating system architecture. Afterwards, simply run the executable installer and follow the instructions.

6. Install everything for *FETranslator*

FETranslator is a *Java*-based tool to translate models between finite element software. *FETranslator* implements the conversion of meshes from commercial FE tools into the format that *Peridigm* is capable of using as a discretization for the creation of peridynamic collocation points.

In order to use the *FETranslator* an implementation of the *Java* Runtime Environment (JRE) is necessary. To translate the mesh into binary format the tool *ncgen* from *NetCDF-C* is required.

6.1. Linux

6.1.1. Java

openSUSE comes with a pre-installed version of the *openJDK* which is a free and open source implementation of the Java Platform, Standard Edition (Java SE). *openJDK* should be perfectly capable of running *FETranslator*. To see if and which version of *Java* is installed on your system open a shell and type:

```
java -version
```

However, since additions and changes to the *FETranslator* can be necessary, a *Java*-capable IDE is required. The Oracle *Java* Development Kit (JDK) offers an integrated solution with the JRE and *NetBeans* as IDE.

6.1.1.1. Install only *Java* development kit (JDK)

1. Go to: <http://www.oracle.com/technetwork/java/javase/downloads/index.html>
2. Click on *Java Platform (JDK)*
3. Accept the License Agreement
4. Open a shell and type `lsb_release -a` and check your operating system architecture (32bit: i586; 64bit: x86_64)
5. Click on the according `rpm` file for your Linux version (here: `jdk-8u91-linux-i586.rpm` for 32bit or `jdk-8u91-linux-x64.rpm` for 64bit, we use 64bit)

6. In the dialog choose *Save File* and save the file somewhere convenient on your system
7. Open a root shell or a normal shell and switch to root user with

```
su -
```

8. Change directory to the folder where the RPM file is located
9. Type

```
zypper install jdk-8u91-linux-x64.rpm
zypper install update-alternatives
update-alternatives --install /usr/bin/java java /usr/java/jdk1.8.0_91/bin/java 1065
update-alternatives --install /usr/bin/javac javac /usr/java/jdk1.8.0_91/bin/javac 1065
update-alternatives --install /usr/bin/jar jar /usr/java/jdk1.8.0_91/bin/jar 1065
update-alternatives --install /usr/bin/javaws javaws /usr/java/jdk1.8.0_91/bin/javaws 1065
update-alternatives --config java
java -version
nedit /home/$USERNAME/.bashrc &
```

10. Add `export JAVA_HOME=/usr/java/jdk1.8.0_91/` to the `.bashrc`-file

6.1.1.2. Install *Java* development kit (JDK) with *NetBeans*

1. Go to: <http://www.oracle.com/technetwork/java/javase/downloads/index.html>
2. Click on *NetBeans with JDK*
3. Accept the License Agreement
4. Open a shell and type `lsb_release -a` and check your operating system architecture (32bit: i586; 64bit: x86_64)
5. Click on the according `sh` file for your Linux version (here: `jdk-8u91-nb-8_1-linux-x64.sh`)
6. In the dialog choose *Save File* and save the file somewhere convenient on your system
7. Open a root shell or a normal shell and switch to root user with

```
su -
```

8. Change directory to the folder where the `.sh` file is located
9. Change the installer file's permissions so it can be executed:

```
chmod u+x <installer-file-name>
```

10. Type

```
./<installer-file-name>
```

11. In the installation wizard:
 - a) At the Welcome page of the installation wizard, click *Next*.
 - b) At the JDK Installation page, specify the directory where to install the JDK, here `/usr/local/java/jdk1.8.0_91`, and click *Next*.
 - c) At the *NetBeans* IDE Installation page, do the following:
 - Specify the directory for the *NetBeans* IDE installation (here `/usr/local/java/netbeans-8.1`)
 - Accept the default JDK installation to use with the IDE or specify another JDK location.
 - d) Accept the default JDK installation to use with the IDE or specify another JDK location.
 - e) Click *Next*
 - f) Review the Summary page to ensure the software installation locations are correct.
 - g) Click *Intall* to begin the installation.
 - h) At the Setup Complete page, provide anonymous usage data if desired, and click *Finish*
 - i) When the installation is complete, you can view the log file, which resides in the following directory: `~/.nbi/log`.

12. Type

```
zypper install update-alternatives
update-alternatives --install /usr/bin/java java /usr/local/java/jdk1
.8.0_91/bin/java 1065
update-alternatives --install /usr/bin/javac javac /usr/local/java/
jdk1.8.0_91/bin/javac 1065
update-alternatives --install /usr/bin/jar jar /usr/local/java/jdk1
.8.0_91/bin/jar 1065
update-alternatives --install /usr/bin/javaws javaws /usr/local/java/
jdk1.8.0_91/bin/javaws 1065
update-alternatives --config java
java -version
nedit /home/$USERNAME/.bashrc &
```

13. Add

```
export JAVA_HOME=/usr/java/jdk1.8.0_91/
```

and

```
export PATH=$PATH:/usr/local/java/netbeans-8.1/bin
```

to the `.bashrc`-file

14. Start a new shell with `su - $USERNAME` and type `java -version` to see if the correct version is active
15. Start a new shell with `su - $USERNAME` and type `netbeans &` to start the IDE
16. Perform update inside the IDE if asked for

If problems occur during any `update-alternatives --install` try

```
update-alternatives --install /usr/bin/java java /usr/local/java/jdk1.8.0_91/bin/java 1
update-alternatives --install /usr/lib64/browser-plugins/javaplugin.so
javaplugin /usr/local/java/jdk1.8.0_91/jre/lib/amd64/libnpjp2.so 1 --
slave /usr/bin/javaws javaws /usr/local/java/jdk1.8.0_91/bin/javaws
update-alternatives --install /usr/bin/javac javac /usr/local/java/jdk1.8.0_91/bin/javac 1 --slave /usr/bin/jar jar /usr/local/java/jdk1.8.0_91/bin/jar
```

Now you can set the *Java* priorities with:

```
update-alternatives --config java
update-alternatives --config javac
update-alternatives --config javaplugin
```

6.1.2. *NetCDF-C*

The *NetCDF-C*-tool *ncgen* is required to convert the ascii mesh file into the binary format readable by *Peridigm*. *NetCDF-C* should already be installed to use *Peridigm*. If the additions to the `PATH`-variable from subsection 3.4.3 are set, no further actions have to be performed.

6.2. Windows

6.2.1. Java

1. Go to: <http://www.oracle.com/technetwork/java/javase/downloads/index.html>
2. Click on *NetBeans with JDK* for Development Kit and Netbeans or just *Java Platform (JDK)*
3. Perform the installation

6.2.2. *NetCDF-C*

To test the *FETranslator* under Windows it is necessary to have *ncgen* available. *ncgen* is available as part of pre-built *NetCDF-C* libraries. To install the latest release

1. Go to: <http://www.unidata.ucar.edu/software/netcdf/>
2. Click *Pre-built Windows Binaries for the latest version of NetCDF-C*
3. Go to *Latest Release (NetCDF-C X.Y.Z)*, here NetCDF-C 4.4.0
4. Download the executable matching your system, here netCDF4.4.0-NC4-64.exe
5. Execute the installer
6. Add the `bin` folder of the installation path, here `D:\Programme\netCDF 4.4.0\` to the Windows `PATH`-Variable:
 - a) Open the *Windows Control Panel* (Systemsteuerung)
 - b) Open *System*
 - c) Click *Advanced System Settings* (Erweiterte Systemeinstellungen)
 - d) In the *Advanced* tab open *Environment Variables*
 - e) Under *User variables for USERNAME* select `PATH`
 - f) Click *Edit*
 - g) Under *Value of the variable* add the path to the `bin` folder of the *NetCDF-C* installation separated by a semicolon (;), here: `;D:\Programme\netCDF 4.4.0\bin\`
 - h) Click *OK* multiple times

Now you can use *ncgen* in a command-window:

```
ncgen.exe -o $OUTPUTFILENAME.g $INPUTFILENAME.g.ascii
```



Bibliography

- [1] Martin Rädcl and Christian Willberg. *PeriDoX*. GitHub repository. Mar. 2018. DOI: [10.5281/zenodo.1403015](https://doi.org/10.5281/zenodo.1403015). URL: <https://github.com/PeriDoX/PeriDoX>.
- [2] Michael L. Parks et al. *Peridigm Users Guide v1.0.0*. Tech. Report SAND2012-7800. Sandia report. Albuquerque, New Mexico 87185 and Livermore, California 94550, USA, 2012. URL: <http://www.sandia.gov/~djlittl/docs/PeridigmV1.0.0.pdf>.
- [3] Larry A. Schoof and Victor R. Yarberry. *Exodus II: A Finite Element Data Model*. SAND92-2137, UC-705. Sandia report. Albuquerque, New Mexico 87185 and Livermore, California 94550, USA, 1994.

Appendices

A. Build-scripts for Libraries

In the following sections, the build scripts for the libraries for *Peridigm* are collected. These are Bash-scripts or *CMake*-files.

The scripts are taken from <https://peridigm.sandia.gov/> and modified slightly if necessary.

The files are provided with UTF-8 encoding. Please modify to your needs if necessary.

A.1. *Boost*

A.1.1. *Boost* 1.55.0

Open a text editor, copy the following code into a file and save as `install_boost-1.55.0.sh`

Listing A.1: Install script for *Boost* 1.55.0

```
# Set environment variables for MPI compilers
export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export F77=mpif77

# Run the Boost bootstrap script
./bootstrap.sh

# add using mpi to user-config.jam
echo "using mpi ;" >> tools/build/v2/user-config.jam
cp tools/build/v2/user-config.jam ~/

# Compile and install Boost using the Boost's bjam build system
./b2 install --prefix=/usr/local/lib/boost-1.55.0/
```

Alternatively, you can [download](#) the script from within this document.

A.1.2. *Boost* 1.60.0

Open a text editor, copy the following code into a file and save as `install_boost-1.60.0.sh`

Listing A.2: Install script for *Boost* 1.60.0

```
# Set environment variables for MPI compilers
export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export F77=mpif77

# Run the Boost bootstrap script
./bootstrap.sh

# add using mpi to project-config.jam
echo "using mpi ;" >> project-config.jam

# Compile and install Boost using the Boost's bjam build system
./b2 install --prefix=/usr/local/lib/boost-1.60.0/
```

Alternatively, you can [download](#) the script from within this document.

A.2. *HDF5*

Open a text editor, copy the following code into a file and save as `install_hdf.sh`

Listing A.3: Install script for *HDF5*

```
# Set environment variables for MPI compilers
export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export F77=mpif77

# Configure HDF5
./configure --prefix=/usr/local/bin/hdf5-1.8.16/ --enable-parallel

# Make and install HDF5
make -j 4
make install
```

Alternatively, you can [download](#) the script from within this document.

A.3. *NetCDF-C*

Open a text editor, copy the following code into a file and save as `install_netcdf.sh`

Listing A.4: Install script for *NetCDF-C*

```
# Set environment variables for MPI compilers
export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export F77=mpif77

# Configure NetCDF
./configure --prefix=/usr/local/bin/netcdf-4.4.0/ --disable-netcdf-4 --
    disable-dap

# Make, test, and install NetCDF
make -j 4
make check
make install
```

Alternatively, you can [download](#) the script from within this document.

A.4. *Trilinos*

Open an editor, copy the following code into the file and save as `cmake_trilinos.cmake`. The final line marks the path to the *Trilinos* source directory, which is named `$DOWNLOAD_DIR` in the documentation.

Listing A.5: *CMake* script for *Trilinos*

```
rm -f CMakeCache.txt
rm -rf CMakeFiles/

cmake -D CMAKE_INSTALL_PREFIX:PATH=/usr/local/bin/trilinos-12.4.2/ \
-D MPI_BASE_DIR:PATH="/usr/local/lib/openmpi-1.10.2/" \
-D CMAKE_CXX_FLAGS:STRING="-O2 -std=c++11 -pedantic -ftrapv -Wall -Wno-
    long-long" \
-D CMAKE_BUILD_TYPE:STRING=RELEASE \
-D Trilinos_WARNINGS_AS_ERRORS_FLAGS:STRING="" \
-D Trilinos_ENABLE_ALL_PACKAGES:BOOL=OFF \
-D Trilinos_ENABLE_Teuchos:BOOL=ON \
-D Trilinos_ENABLE_Shards:BOOL=ON \
-D Trilinos_ENABLE_Sacado:BOOL=ON \
```

```

-D Trilinos_ENABLE_Epetra:BOOL=ON \
-D Trilinos_ENABLE_EpetraExt:BOOL=ON \
-D Trilinos_ENABLE_Ipack:BOOL=ON \
-D Trilinos_ENABLE_AztecOO:BOOL=ON \
-D Trilinos_ENABLE_Amesos:BOOL=ON \
-D Trilinos_ENABLE_Anasazi:BOOL=ON \
-D Trilinos_ENABLE_Belos:BOOL=ON \
-D Trilinos_ENABLE_ML:BOOL=ON \
-D Trilinos_ENABLE_Phalanx:BOOL=ON \
-D Trilinos_ENABLE_Intrepid:BOOL=ON \
-D Trilinos_ENABLE_NOX:BOOL=ON \
-D Trilinos_ENABLE_Stratimikos:BOOL=ON \
-D Trilinos_ENABLE_Thyra:BOOL=ON \
-D Trilinos_ENABLE_Rythmos:BOOL=ON \
-D Trilinos_ENABLE_MOOCHO:BOOL=ON \
-D Trilinos_ENABLE_TriKota:BOOL=OFF \
-D Trilinos_ENABLE_Stokhos:BOOL=ON \
-D Trilinos_ENABLE_Zoltan:BOOL=ON \
-D Trilinos_ENABLE_Piro:BOOL=ON \
-D Trilinos_ENABLE_Teko:BOOL=ON \
-D Trilinos_ENABLE_SEACASioss:BOOL=ON \
-D Trilinos_ENABLE_SEACAS:BOOL=ON \
-D Trilinos_ENABLE_SEACASblot:BOOL=ON \
-D Trilinos_ENABLE_Pamgen:BOOL=ON \
-D Trilinos_ENABLE_EXAMPLES:BOOL=OFF \
-D Trilinos_ENABLE_TESTS:BOOL=ON \
-D TPL_ENABLE_Matio:BOOL=OFF \
-D TPL_ENABLE_HDF5:BOOL=ON \
-D HDF5_INCLUDE_DIRS:PATH="/usr/local/bin/hdf5-1.8.16/include" \
-D HDF5_LIBRARY_DIRS:PATH="/usr/local/bin/hdf5-1.8.16/lib" \
-D TPL_ENABLE_Netcdf:BOOL=ON \
-D Netcdf_INCLUDE_DIRS:PATH="/usr/local/bin/netcdf-4.4.0/include" \
-D Netcdf_LIBRARY_DIRS:PATH="/usr/local/bin/netcdf-4.4.0/lib" \
-D TPL_ENABLE_MPI:BOOL=ON \
-D TPL_ENABLE_BLAS:BOOL=ON \
-D TPL_ENABLE_LAPACK:BOOL=ON \
-D TPL_ENABLE_Boost:BOOL=ON \
-D Boost_INCLUDE_DIRS:PATH="/usr/local/lib/boost-1.55.0/include" \
-D Boost_LIBRARY_DIRS:PATH="/usr/local/lib/boost-1.55.0/lib" \
-D CMAKE_VERBOSE_MAKEFILE:BOOL=OFF \
-D Trilinos_VERBOSE_CONFIGURE:BOOL=OFF \
/usr/local/src/trilinos-12.4.2-Source/

```

Alternatively, you can [download](#) the script from within this document.

A.5. *Peridigm*

A.5.1. CMake script for *Peridigm*

Open an editor, copy the following code into the file and save as `cmake_peridigm.cmake`. The final line marks the path to the *Peridigm* source directory, which is named `$DOWNLOAD_DIR` in the documentation.

Listing A.6: CMake script for *Peridigm*

```
rm -f CMakeCache.txt
rm -rf CMakeFiles/

cmake \
-D CMAKE_BUILD_TYPE:STRING=Release \
-D Trilinos_DIR:PATH=/usr/local/bin/trilinos-12.4.2/lib/cmake/Trilinos/ \
-D CMAKE_C_COMPILER:STRING=/usr/local/lib/openmpi-1.10.2/bin/mpicc \
-D CMAKE_CXX_COMPILER:STRING=/usr/local/lib/openmpi-1.10.2/bin/mpicxx \
-D BOOST_ROOT=/usr/local/lib/boost-1.55.0/ \
-D CMAKE_CXX_FLAGS:STRING="-O2 -Wall -std=c++11 -pedantic -Wno-long-long
  -ftrapv -Wno-deprecated" \
/usr/local/src/Peridigm-1.4.1-Source
```

Alternatively, you can [download](#) the script from within this document.

A.5.2. Script for cloning *Peridigm* from GitHub and compiling on the STM-Cluster

Listing A.7: Script for cloning *Peridigm* from GitHub and compiling on the STM-Cluster

```
#!/bin/bash

#####
# Header                                     #
#####
#
# Install Peridigm from github repository master
#
# Requirements:
#             Allocate exclusive node before using this script:
#             salloc --exclusive
#
# Revisions: 2017-12-22 Martin Raedel <martin.raedel@dlr.de>
#             Initial draft
```

```

#
# Contact:   Martin Raedel,  martin.raedel@dlr.de
#           DLR Composite Structures and Adaptive Systems
#
#           _ _/|_ _
#           / _/ _/ _/
#           www.dlr.de/fa/en      | / DLR
#
#####
# Content                                     #
#####

#-----
# Variables
#-----

# The directory where all the magic happens - should not exist in advance
basedir=$HOME'/Documents/Peridigm/20171222EC_/'

# Path from where to clone
githubclonepath='https://github.com/peridigm/peridigm.git'

# Internal directory names
builddir='build'
srcdir='src'

# File names
file_cmake='cmake_peridigm.cmake'
file_cmake_log='cmake_peridigm.log'
file_make_log='make.log'
file_make_test_log='make_test.log'
file_make_install_log='make_install.log'

file_peridigm_bin='Peridigm'

# Number of CPUs for make
make_cpus = 8

#-----
# Script
#-----

#-----
# Load build environment

```

```

#-----

echo 'Load build environment'
. /cluster/software/slurm/etc/env.d/mpibuild.sh
. /cluster/software/slurm/etc/env.d/peridigm.sh

#-----
# Folder structure
#-----

echo 'Create directory structure'
if [ -d ${basedir} ]; then # Control will enter here if $DIRECTORY doesn
    't exist.
    echo 'Directory '${basedir}' already exists. Exit.'
    exit 0
fi

mkdir ${basedir}
cd ${basedir}
mkdir ${builddir}
mkdir ${srcdir}
cd ${srcdir}

#-----
# Clone from GitHub
#-----

echo 'Clone from GitHub'
git clone ${githubclonepath}
cd ../${builddir}

#-----
# Create cmake file
#-----

echo 'Create and execute cmake file'

# Fill file
echo 'rm -f CMakeCache.txt' >> ${file_cmake}
echo 'rm -rf CMakeFiles/' >> ${file_cmake}
echo '' >> ${file_cmake}
echo 'cmake \' >> ${file_cmake}
echo '-D CMAKE_BUILD_TYPE:STRING=Release \' >> ${file_cmake}
echo '-D CMAKE_INSTALL_PREFIX='${basedir}${builddir}' \' >> ${file_cmake}

```

```

echo '-D CMAKE_CXX_FLAGS:String="-O2 -Wall -std=c++11 -pedantic -Wno-long
      -long -ftrapv -Wno-deprecated" \' >> ${file_cmake}
echo ${basedir}${srcdir}/peridigm/' >> ${file_cmake}

# Change permissions to make cmake-file executable
chmod u+x ${file_cmake}

# Execute cmake-file
./${file_cmake} > ${file_cmake_log} 2>&1

#-----
# Make
#-----

echo 'make'
make -j ${make_cpus} > ${file_make_log} 2>&1

echo 'make test'
make test > ${file_make_test_log} 2>&1
if grep -q Error ${file_make_test_log}; then
    echo '  make test contains failed tests'
else
    echo '  all tests passed'
fi

echo 'make install'
make install > ${file_make_install_log} 2>&1

#-----
# Comment
#-----

cd bin
echo 'Finished - Peridigm executable path':
readlink -f ${file_peridigm_bin}

#-----
# Clean
#-----

```

Alternatively, you can [download](#) the script from within this document.

A.6. Make a script executable

In order to use a script file in the shell for installation you must first make the text file executable. Therefore, open a terminal, change directory to the folder the individual script is located and make the script executable for the user with

```
chmod u+x $SCRIPTNAME.sh
```

A.7. Modifications of `.bashrc`

When an interactive shell that is not a login shell is started, `bash` reads and executes commands from `~/.bashrc`, if that file exists. You can find the `.bashrc` file in your user home directory `/home/$USER/` with `ls -al`.

The following listings shows a modified `.bashrc` file which includes the exportation of the significant libraries in the `$PATH` and `$LD_LIBRARY_PATH` environment variables. The header is not printed.

Be aware:

- In case you use a 32bit operating system, or in some cases also for 64bit operating system, the `lib64`-folders must be changed to `lib`.
- The entries to the `$PATH` and `$LD_LIBRARY_PATH` variables should be added step-by-step **after** the installation of the individual tool. Otherwise, the install scripts might find pre-compiled items and use these instead of creating new binaries with the current settings.

A.7.1. `.bashrc` for *Peridigm* 1.4.1

Listing A.8: Modified `.bashrc`-file to set environment variables for *Peridigm* 1.4.1

```
test -s ~/.alias && . ~/.alias || true

# add default lib paths
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/lib
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/lib64
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib64

# add cmake
export PATH=$PATH:/usr/local/bin/cmake-3.4.3/bin

# add openMPI
```



```
export PATH=$PATH:/usr/local/lib/openmpi-1.10.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/openmpi-1.10.2/
lib64

# add boost
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/boost-1.55.0/lib

# add hdf5
export PATH=$PATH:/usr/local/bin/hdf5-1.8.16/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/hdf5-1.8.16/lib64

# add netcdf
export PATH=$PATH:/usr/local/bin/netcdf-4.4.0/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/netcdf-4.4.0/lib64

# add trilinos
export PATH=$PATH:/usr/local/bin/trilinos-12.4.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/trilinos-12.4.2/
lib
```

You can [download](#) the file from within this document.

A.7.2. .bashrc for *Peridigm* 1.5

Listing A.9: Modified .bashrc-file to set environment variables for *Peridigm* 1.5

```
test -s ~/.alias && . ~/.alias || true

# add default lib paths
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/lib
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/lib64
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib64

# add cmake
export PATH=$PATH:/usr/local/bin/cmake-3.5.1/bin

# add openMPI
export PATH=$PATH:/usr/local/lib/openmpi-1.10.2/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/openmpi-1.10.2/lib

# add boost
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/lib/boost-1.60.0/lib
```

```
# add hdf5
export PATH=$PATH:/usr/local/bin/hdf5-1.8.16/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/hdf5-1.10.0/lib64

# add netcdf
export PATH=$PATH:/usr/local/bin/netcdf-4.4.0/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/netcdf-4.4.0/lib64

# add trilinos
export PATH=$PATH:/usr/local/bin/trilinos-12.6.1/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/bin/trilinos-12.6.1/
lib
```

You can [download](#) the file from within this document.

B. FAQ

The error `g++ internal compiler error killed (program cc1plus)` occurs while compiling with `make -j N`. What is that?

- The problem is probably caused by insufficient memory.
- Try typing `free -m` in a terminal while compiling to see the amount of free RAM
- Running `make -j 4` runs lots of process which use more memory. The problem above occurs when your system runs out of memory. In this case rather than the whole system falling over, the operating systems runs a process to score each process on the system. The one that scores the highest gets killed by the operating system to free up memory. If the process that is killed is `cc1plus`, `gcc` (perhaps incorrectly) interprets this as the process crashing and hence assumes that it must be a compiler bug. But it isn't really, the problem is the OS killed `cc1plus`, rather than it crashed.
- If this is the case, you are running out of memory. So run perhaps `make -j 2` instead. This will mean fewer parallel jobs and will mean the compilation will take longer but hopefully will not exhaust your system memory.

When I call `make test` after the *Peridigm* installation all multi-processor-tests fail. What is the problem?

- Make sure you do not execute `make test` as root user. It is not allowed to call `mpirun` as root. If you call `mpirun` as root, the job is cancelled automatically.
- In order to run the tests as a normal user make sure you set the permissions of the *Peridigm* installation folder to allow execution for group and others

Everything works fine, all *Peridigm* tests are passed, but when I call *decomp* I get a `*HDF5 library version mismatched error***` error. Why?**

- It seems *decomp* finds another version of the *HDF5* library `libhdf5.so` than the one you use to compile *Trilinos* with.
- This can be caused by installation of other tools via the *YaST2* software management which puts libraries in `/usr/lib` or `/usr/lib64`. These are found in the current `LD_LIBRARY_PATH` before the *HDF5* version installed in this guide.
- Tools which bring their own version of *HDF5* are for example:

Tool/Package	<i>HDF5</i> version
octave-forge-netcdf	1.8.15
- If these packages are installed and you do not use them, uninstall them and the *HDF5* libraries as described in subsection 3.3.2. You do not have to recompile anything. Just try using *decomp* afterwards.
- In case you really really need the tool with the other *HDF5* there seems to be nothing left to to but to compile *Trilinos* using this version of *HDF5*.

I get errors when using the provided CMake-files, like [...] command not found.
What can I do?

- This problem may arise if you import the appended scripts under Windows.
- The end-of-line character might be changed to CR-LF instead of LF
- To check this problem, open *Notepad++* and go to *Edit* → *EOL Conversion* → *Convert to Unix Format (LF)*
- Save and try using the script again

C. Non-necessary tools & scripts

The installation is described for *openSUSE* for version 42.1.

C.1. *NEdit*

NEdit, the Nirvana editor, is a text editor and source code editor for the X Window System. For the installation of the editor *NEdit* visit:

<http://software.opensuse.org/download.html?project=editors&package=nedit>

You can either choose the 1-Click-installation or add the repository and install manually. For the latter login to a terminal as **root** and type

```
zypper addrepo http://download.opensuse.org/repositories/editors/
    openSUSE_Leap_42.1/editors.repo
zypper refresh
zypper install nedit
```

C.2. RM- \LaTeX

Download the package via the intranet (from within the DLR network or via a VPN connection):

<teamsites.dlr.de/rm/latex/SitePages/Homepage.aspx>

Follow the instructions given in `/doc/RM-LaTeX-Guide/RM-LaTeX-Guide.pdf`.

C.2.1. Linux

Before using `mktexlsr` set

```
chmod +t texmf/
```

and

```
chmod go+w texmf/
```

Due to some problems in the RM-L^AT_EX package meaningful use is only possible under Windows. If using with Linux do not use everything related to the package `dlrsecondpage`.

C.2.2. Windows

There should be no additional steps necessary.

D. This document

D.1. Repository

This document is part of the PeriDoX repository. The complete repository can be found at:

<https://github.com/PeriDoX/PeriDoX>

D.2. Typesetting

This document was originally typeset using the documentclass `dlrreprt` from the DLR-internal RM- \LaTeX package.

The RM- \LaTeX package is not publicly available. Therefore, this document is compatible with a bootstrap-version of the documentclass, called `bootstrap_dlrreprt`. `bootstrap_dlrreprt` class is part of this repository.

The compilation is performed with `pdflatex` with the following options:

```
pdflatex --shell-escape -synctex=1 -interaction=nonstopmode %source --  
extra-mem-top=60000000
```

The bibliography is compiled with `biber`. The glossary must be compiled with `makeindex` or, for Windows, the included batch-script may be used. The keyword index is created automatically.

The general compilation order is:

```
pdflatex → biber → makeindex → pdflatex → pdflatex
```

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